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16. ABSTRACT

The Empirical Kinetic Modeling Approach (EKMA) was evaluated using the results of model applications in the Philadelphia area, primarily by comparing results of the box model (OZIPM) that forms the basis of the EKMA with those of more sophisticated models. The study was carried out at several levels, beginning with evaluation of OZIPM and ending with an evaluation of the control strategy predictions resulting from use of the EKMA isopleth methodology. OZIPM results were compared with those of the Urban Airshed Model (UAM), which is listed as one of the EPA's preferred models, and the Systems Applications Trajectory models, as well as with those obtained with modified versions of the original OZIPM model. The basic OZIPM model is a simple moving air parcel, or box, model that uses a detailed chemical mechanism for surrogate propylene and butane hydrocarbons. The model treats time-dependent precursor-emission factors and expansion of the air parcel. Entrainment is treated by assuming that constant concentrations exist outside the parcel. The primary emphasis of this comparison study was identification of features in the basic OZIPM model that could explain differences between the results of the OZIPM model and those of other models.

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APPLICATION OF THE EMPIRICAL KINETIC MODELING APPROACH TO URBAN AREAS

Volume III: Philadelphia

By

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U.S. ENVIRONMENTAL PROTECTION AGENCY
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October 1985

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1 INTRODUCTION

BACKGROUND AND OBJECTIVES

For several years the Office of Research and Development of the U.S. Environmental Protection Agency (EPA) has sponsored a coordinated program consisting of fundamental chemical research, smog chamber experimentation, and model development. The objective of this program is to develop mathematical models capable of simulating the dynamics of the chemical reactions, and the dispersion of the gaseous pollutants, found in the lower troposphere. These atmospheric models will be used both to gain an understanding of air pollution and to predict the probable outcome of air pollution control scenarios. To this end, the EPA Office of Air Quality Planning and Standards (OAQPS) has embarked on an extensive program of model comparison and evaluation.

The specific purpose of the OAQPS program is to assess the suitability of available photochemical oxidant modeling approaches for use by states as planning tools in ozone air quality planning and management. The program includes comparisons and evaluations of various approaches for typical United States cities. As part of the program, large, detailed data bases are being assembled for several example cities.

The primary objective of this report is to evaluate the Empirical Kinetics Modeling Approach (EKMA) through application of the photochemical box model (OZIPM) that forms its basis. Because some models are grid-based and thus designed to reproduce spatial and temporal variations within the metropolitan airshed, detailed information files are required. The EPA has prepared highly detailed data concerning precursor emissions, meteorology, and ambient air quality for the cities of Tulsa and Philadelphia to test various air quality simulation models such as OZIPM and the Urban Airshed Model (UAM). In addition, data bases are already available for St. Louis, Los Angeles, San Francisco, and Sacramento. The availability of detailed data and the results of parallel studies using sophisticated models offer the following advantages for an in-depth study of EKMA:

(1) The simple application of the OZIPM box model, using either the actual available data inputs or the corresponding data simulated by other models, should generate results that can be compared both with ambient air data and with the results of the other models. The timing of results regarding the ozone maxima and precursor decay should also be comparable.

(2) Tests of the sensitivity of the results to variations in the input data can demonstrate important data requirements for successful application of OZIPM. This information should be useful in determining its cost effectiveness for future uses. The results of the sensitivity study will also be useful for improving OZIPM in case the present version does not adequately simulate observed ambient data or the simulations of more complex models.

(3) The application of the EKMA procedures to air quality planning demonstrates its utility compared with that of methods based either on simpler models or on more complex models (such as the UAM).

(4) The potential effectiveness of OZIPM model improvements can be assessed using the results of the complex models as a standard.

THE EMPIRICAL KINETIC MODELING APPROACH

The EPA has developed a method for estimating the emission controls needed to meet the National Ambient Air Quality Standard (NAAQS) for ozone (O_3) concentrations in urban areas. This method, known as the Empirical Kinetic Modeling Approach (EKMA), uses an isopleth diagram of ozone concentrations that is related to hydrocarbon (HC) and nitrogen oxide (NO_x) precursor levels. Each point on the isopleth diagram represents the maximum one-hour ozone level reached as a result of the specific HC and NO_x combination described by the abscissa and ordinate values of the isopleth diagram. The ozone value generated from each HC and NO_x combination is obtained by means of a computer-based trajectory model--the Ozone Isopleth Plotting Package (OZIPP) (Whitten and Hogo, 1978) and OZIPM for alternate chemical mechanisms (EPA, 1984). The OZIPM trajectory model contains many simplifying assumptions and options that are designed to strike a balance between factors such as the state of knowledge, data availability, computer size, predictive accuracy, and overall cost.

AN OVERVIEW OF EKMA COMPARISON EVALUATIONS

Four studies have been performed by Systems Applications to evaluate the EKMA through comparison of the results of OZIPM trajectory model with those of other models. Three of these four studies were sponsored by the EPA; the Philadelphia study is the third of the three. The first study compared the UAM and the Systems Applications Trajectory models with various versions of the box model used in EKMA for the Los Angeles area (Whitten and Hogo, 1981). In the second study, the LIRAQ model formed the basis for the San Francisco area comparison, and the Systems Applications models were used for the Sacramento area (Whitten et al., 1981). The UAM was also used in the study of the Tulsa area and for this study of the Philadelphia area.

A comparison evaluation is performed at several levels to provide a spectrum of information. The independent application of the EKMA-OZIPM in areas where other models have been applied merely validates the common assumption that different models can sometimes produce different results. In addition, this study attempts to provide information explaining why specific features of the different models lead to different results. For instance, a specific feature of grid models (in contrast to trajectory models in general) is their ability to simulate some wind shear effects. Grid and trajectory models have been found to produce different results when wind shear effects are significant; the reverse is also true (similar results can occur when wind shear is minimal). Thus, specific model differences can be associated with differences in results. Given the previous example, a prospective user should apply the trajectory model with a measure of discretion in situations known to have a high wind shear.

Different levels of evaluation are possible within the EKMA framework. The control scenario estimations generated by EKMA isopleth diagrams are the end result of a series of steps involving model assumptions and adjustments. The basis of the EKMA is a trajectory model, which is quite simple from the standpoint of dispersion. This trajectory model can be applied in the absolute sense as an atmospheric model on its own. The OZIPM computer code that contains this model also has an array of options, each of which will be geared to some specific standardized setting if the user does not exercise this option.

The isopleth diagram is used in a relative manner, so that if all the options and inputs fail to generate a simulated ozone value that agrees with observations, the final discrepancy is eliminated by using the observed value. Some discrepancy is almost always expected because, except for the chemistry employed, the EKMA-OZIPM is a rather simplistic approach.

The use of the observed ozone value rather than the simulated value is intended to account for some of the simplifications inherent in the EKMA-OZIPM.

The levels of evaluation in this study begin with the specific features that define each basic model; other levels involve input data and options. At each level, the present study attempts to make comparisons with other models, observations, and alternate methodologies. However, the evaluation of atmospheric models does not necessarily fit a specific, well-organized framework. Problems that are unique to some areas are not always apparent ahead of time. Thus, the study of the Philadelphia area reported here is only part of an overall evaluation of the EKMA. The following sections present the specific results and analysis of the Philadelphia study as they relate to the EKMA evaluation.

SECTION 2

MODEL APPLICATIONS

This section describes the photochemical air quality models used in this study and the inputs associated with each model. Descriptions of the Philadelphia study region and the modeling days used in that study are also presented. As noted, the purpose of this study is to compare the ozone predictions of air quality models of different complexity (in particular, to compare EKMA calculations with current UAM applications). These models can be classified on the basis of their complexity according to the levels of analysis described in the 1979 Federal Register (65669-65670) on ozone modeling:

Level I: Sophisticated dispersion models such as the Urban Airshed (UAM) and Systems Applications' Trajectory models.

Level II: Box models such as OZIPM/CBM.

Level III: The city-specific EKMA.

Level IV: The standard EKMA.

The UAM is a three-dimensional grid model that mathematically simulates the physical and chemical processes responsible for photochemical smog. One of the advantages offered by a three-dimensional grid model is the ability to consider spatial and temporal effects of control strategies, whereas models of less complexity consider temporal effects only. The structure of the UAM consists of an array of cells, the total volume of which represents an urban area. The horizontal dimensions of each cell are constant, but the vertical thickness of the cells vary according to the depth of the mixed layer and top of the boundary region throughout the simulation. The UAM can simulate the advection of pollutant species through the modeling region, the diffusion of material from cell to cell, the injection of primary source emissions into the modeled region, and the chemical transformations of reactive species into intermediate and secondary products.

The UAM was applied to Philadelphia for two days in 1979--13 July and 19 July--to compare model predictions with station observations. The model was then used to evaluate ozone control requirements for the Philadelphia area. The inputs to the UAM served as a data base for the series of less complex models. Descriptions of each model are presented in the following sections followed by a summary of UAM inputs (described in detail in the Appendix). Inputs to the less complex models are also presented.

DESCRIPTION OF THE MODELS USED IN THIS STUDY

The following models were used in this study:

The Urban Airshed Model (UAM)--a three-dimensional grid model that uses CBM-II chemistry.

The Systems Applications Trajectory Model--In terms of inputs, computations, and results at points along a selected trajectory, this model differs from the UAM only in the elimination of horizontal dispersion and vertical winds.

Level II box model (OZIPM/CBM)--uses the same meteorological inputs as the Systems Applications Trajectory Model, but also uses both the CBM-II and the CBM-III chemistry.

The level III city-specific OZIPM model--uses Carbon-Bond chemistry as described by EPA (1984) and the standard EKMA chemistry as described by EPA (1981).

In this section, the principal differences among these models are highlighted.

Comparison of the Urban Airshed and Systems Application Trajectory Models*

These two models were designed to complement each other; therefore, many algorithms are identical for both models (several subroutines of the computer codes are actually shared). Furthermore, the models use the same input files. The trajectory model begins on a square of the grid model at a specific time. The path of the trajectory is then determined solely by the wind speed and direction in the lowest level, or some average of the

---

* Detailed discussions of this comparison are available elsewhere (see Reynolds et al., 1979).

lowest two levels, of the grid-model input files. Because the other levels in the grid model often advect with velocities that are different from the lowest level, the two models often generate different results as the simulations progress in time. Nevertheless, the trajectory model provides an inexpensive means of evaluating parts of the grid model at specific locations and times.

A special feature of the trajectory model is its ability to be operated backward in time. This feature was used to generate the trajectories used in this study. The time and location of either the observed or the simulated ozone maximum were used to start the backward trajectory to 0500 EDT. Thus, the forward trajectories always arrived at the desired spot at the proper time for comparison with either observations or grid-model results. Changes in emissions often lead to changes in the time and location of maximum ozone concentrations. Small changes in times of maximum ozone concentration at some specific monitoring site can be associated with rather large differences in the location of the origin of, and in the actual pathway taken by, the air parcel producing the specific ozone maximum. Therefore, when compared with a grid model, any trajectory model used as a tool for control strategies possesses the inherent shortcoming of being incapable of accounting for these changes.

Comparison of the Systems Applications Trajectory Model and the OZIPM/CBM Model

The following similarities and differences exist between the Systems Applications' Trajectory model and the level II OZIPM/CBM:

Chemistry. Both of these models employ CBM-II chemistry, which is also used in the UAM. However, the photolytic constants are computed differently in the OZIPM/CBM than in the UAM and Trajectory models. In order to compare different models, the same data base is needed and the chemistry used in the models must be as similar as possible so that any differences in the results can be attributed to individual model characteristics and not the differences in the chemistry. The NO_2 photolysis rates normally used in the OZIPM/CBM are somewhat lower than those used in the UAM and Trajectory models, which are based on actual measurements. Therefore, for this study the OZIPM/CBM values were modified for NO_2 photolysis using a constant factor so that all models agreed at 1300 EDT.

In the UAM and Trajectory models, the rates of all other photolytic reactions vary with NO_2 photolysis, with a fixed ratio for each, whereas in the OZIPM/CBM the photolysis rates vary independently.

Aldehyde photolysis was adjusted in the OZIPM/CBM to provide agreement between the models at 1100 EDT. Actually, these differences in photolysis rates with zenith angle constitute an advantage in sophistication for the OZIPM/CBM.

The use of fixed ratios to NO_2 photolysis in the Systems Applications models, in place of the variable ratios used in the OZIPM/CBM model can lead to minor differences in chemistry. The ratios are at a maximum at solar noon and a minimum at sunrise and sunset (Whitten et al., 1980). The photolysis rates for aldehydes change more with solar zenith angle than the NO_2 photolysis rate does because aldehydes photolyze at the short wavelength end of the solar spectrum, whereas NO_2 photolyzes nearer the long wavelength end of the ultraviolet spectrum. The short ultraviolet wavelengths are more affected by the ozone in the stratosphere than are the longer wavelengths. At high zenith angles (morning and evening), the solar rays must pass through a thicker layer of ozone. Therefore, the ratio of aldehyde photolysis to NO_2 photolysis varies throughout the day, reaching a maximum at solar noon. For this particular study, the OZIPM/CBM aldehyde photolysis values were multiplied by a constant value throughout each day so that the models agree at 1100 EDT. Therefore, in the early morning the photolysis rate of the aldehydes in the OZIPM/CBM would be somewhat less than that used in the Systems Applications models.

For this particular study, we chose to modify the OZIPM/CBM to make it as much like the UAM and Trajectory models as possible. By removing all possible potential variables between models, we hoped to be able to better compare the fundamentals underlying these models. The CBM version of OZIPM has normally been applied in order to assist users of the Airshed Model to estimate potential control scenarios. For such applications the photolysis adjustments discussed here are normal.

Reactivity. The Systems Applications Trajectory and Airshed models are operated with reactivity splits that vary with each source category. However, the OZIPM/CBM does not have this feature; instead, reactivity is assumed to be constant throughout the day. The OZIPM computer code can accept four different hydrocarbon reactivities: one for background; one for the initial conditions; one for the aged hydrocarbons aloft; and one for the emissions that occur throughout the day. Hence, the only differences in reactivity between models were in the temporal variations aloft and in the variable emissions

used in the Systems Applications models compared with the fixed reactivities employed in the emissions for the OZIPM models. The reactivities used in the OZIPM/CBM were determined from averages of emissions used in the Trajectory model; for averaging the hydrocarbons aloft, a weighting factor was used each hour that was equal to the positive change in mixing height.

In a sense, the NO_2/NO_x ratio also acts as a reactivity effect. The OZIPM/CBM uses a fixed ratio of NO_2/NO_x (10 percent) for all NO_x emissions, whereas the Systems Applications models allow this ratio to vary according to their source category (the average ratio is typically about 5 percent). At this time, it has not been attempted to change the OZIPM/CBM or to fix the ratio in the Systems Applications models, because it is felt that the difference is trivial. For NO_x aloft, the OZIPM/CBM uses pure NO_2, which is close to typical values found in the Trajectory Model simulations because the NO_2/NO_x ratio is almost always greater than 0.85; the values aloft are often greater than 0.99.

Integration Scheme. The OZIPM/CBM uses a Gear-type method without any steady-state approximations, whereas the Trajectory Model uses the same Crank-Nicholson finite-differencing scheme and steady-state approximations that are used in the Airshed Model. However, our previous tests using smog ch[illegible]er experiments suggest that the differences introduced by the numerical integration schemes should be minimal if the steady-state species are carefully chosen.

Vertical Layers. The UAM and Trajectory models share the same vertical layers and algorithms for numerical integration, but additional vertical contributions are introduced into the UAM for convergent or divergent winds. The OZIPM/CBM is limited to providing calculations of the mixed layer as a whole, but fixed concentrations in the layer aloft can be introduced as the mixing height rises. The Systems Applications models account for mixing within the mixed layer, mixing within the inversion layer, and eddy diffusion among all layers. The OZIPM/CBM assumes instantaneous mixing within the entire mixed layer, and no eddy diffusion is considered across the boundary defined by the mixing height.

In our comparison studies, the effectiveness of multilayers and eddy diffusion was one of the central issues to be evaluated in this region of our model series. A problem to avoid, which does confound the comparison, is the entrainment of pollutants from aloft. The OZIPM/CBM requires fixed concentrations aloft, so these must be chosen from some "proper" average of the time-dependent concentrations computed in the Systems Applications Trajectory Model. With

the average value used in this study, the concentrations entrained when the mixing height rises most significantly were weighted most heavily. The concentration entrained was weighted using the ratio of the change in the mixing height per hour to the total change in the mixing height per day. A more complex weighting scheme might involve the time when the greatest effect on the chemistry occurs; however, this effect was not evaluated. Concentrations aloft are not considered for the time before the inversion rises or after it has reached some maximum. As the mixing lid drops late in the afternoon, the only process affecting the surface layer from concentrations aloft is eddy diffusion. Eddy diffusion is treated in the UAM and Trajectory models, but is neglected in the OZIPM/CBM.

Mixing height. All algorithms used in the OZIPM/CBM, as well as those used in the UAM and Trajectory models, can use identical mixing heights with values that vary linearly in time between specified values at each hour.

Temperature. The temperature varies in the UAM and Trajectory models vertically, but the OZIPM/CBM currently employs a fixed temperature for each hour. This difference can be significant. Temperature affects both vertical diffusion and chemistry in the Systems Applications models, but it can affect only chemistry in the OZIPM/CBM because vertical mixing is assumed to occur instantaneously within the mixed layer.

Emissions. Both the UAM and the Systems Applications Trajectory models allow for emissions into all layers. The OZIPM/CBM, however, treats all emissions in the mixing layer alike and does not directly address emissions above the mixing layer. In the OZIPM/CBM, emissions in the layer aloft must be accounted for in the determination of the fixed concentrations aloft. Normally, the OZIPM computer code treats emissions as a multiple of the initial conditions. However, since the sum of the emissions in the lower layers of the Systems Applications' Trajectory model was used for the emissions in the mixing layer in the OZIPM/CBM, the OZIPM code was modified to treat the emissions in an absolute manner. This modification was implemented by using the transported surface layer inputs as the initial concentrations and was done primarily for ease of comparison. The normal initial concentrations (the CALC mode in OZIPM) were specified as 1.0 for both HC and NO_x, but these values were not added as initial concentrations. They were used only for emission fraction development because emissions are expressed relative to these values in the OZIPM code.

Emissions for the Systems Applications Trajectory models are given as total moles emitted into each cell during each hour. To arrive at

values appropriate for the OZIPM/CBM, we used the following conversion procedure: the mixing volumes of the Trajectory Model and the OZIPM/CBM were assumed to be equal below the mixing height, such that

$$V = A \times Z_{mix} \quad ,$$

where A is the area of the horizontal cross-section of the air parcel defined in Trajectory Model simulations and Z_{mix} is the mixing height. If the volume is expressed in cubic centimeters, the moles emitted in one hour (the number available from the Trajectory Model computer output) can be divided by this volume to give moles/cm^3 units. This, in turn, can readily be converted to the OZIPM/CBM units of concentration (ppm) by using a conversion factor of 2.445×10^{10} ppm $moles^{-1}$ cm^3, which is technically correct for a perfect gas at 298 K and 1 atmosphere of pressure. The numbers calculated at this point are almost directly applicable to the OZIPM/CBM model. First, the use of 1.0 for the initial concentrations of HC and NO_x in the CALC mode implies that each one-hour emission number would be the concentration added during the hour if the mixing height were the same as the initial value Z_0. However, the computer codes are written so that, at each instant in time, the emission factor is multiplied by Z_0/Z_{mix}. Therefore, the Z_{mix} drops out and the actual numbers (E_n) used are

$$En = A \times 2.445 \times 10^{10}/Z_0 \quad ,$$

where A and Z_0 are expressed in centimeters.

DESCRIPTION OF THE PHILADELPHIA MODELING REGION

The Philadelphia metropolitan area is not an isolated "airshed" like the Tulsa region; rather, it is nested in the expansive Northeast Urban Corridor. The local ambient ozone levels recorded on a particular day in Philadelphia may be partly the result of the influx of ozone precursors from the New York metropolitan area to the northeast or from the Baltimore/Washington D.C. urban area to the southwest. The Philadelphia area is shown in Figures 1 and 2. Much of the detailed UAM modeling descriptions and results are presented by Braverman and Haney (1985). This section and the appendix summarize the UAM study for the Philadelphia area.

CHARACTERIZATION OF THE PHILADELPHIA MODELING DAYS

From the Philadelphia oxidant data study performed during the summer of 1979, two days were chosen for the validation of the UAM. This section

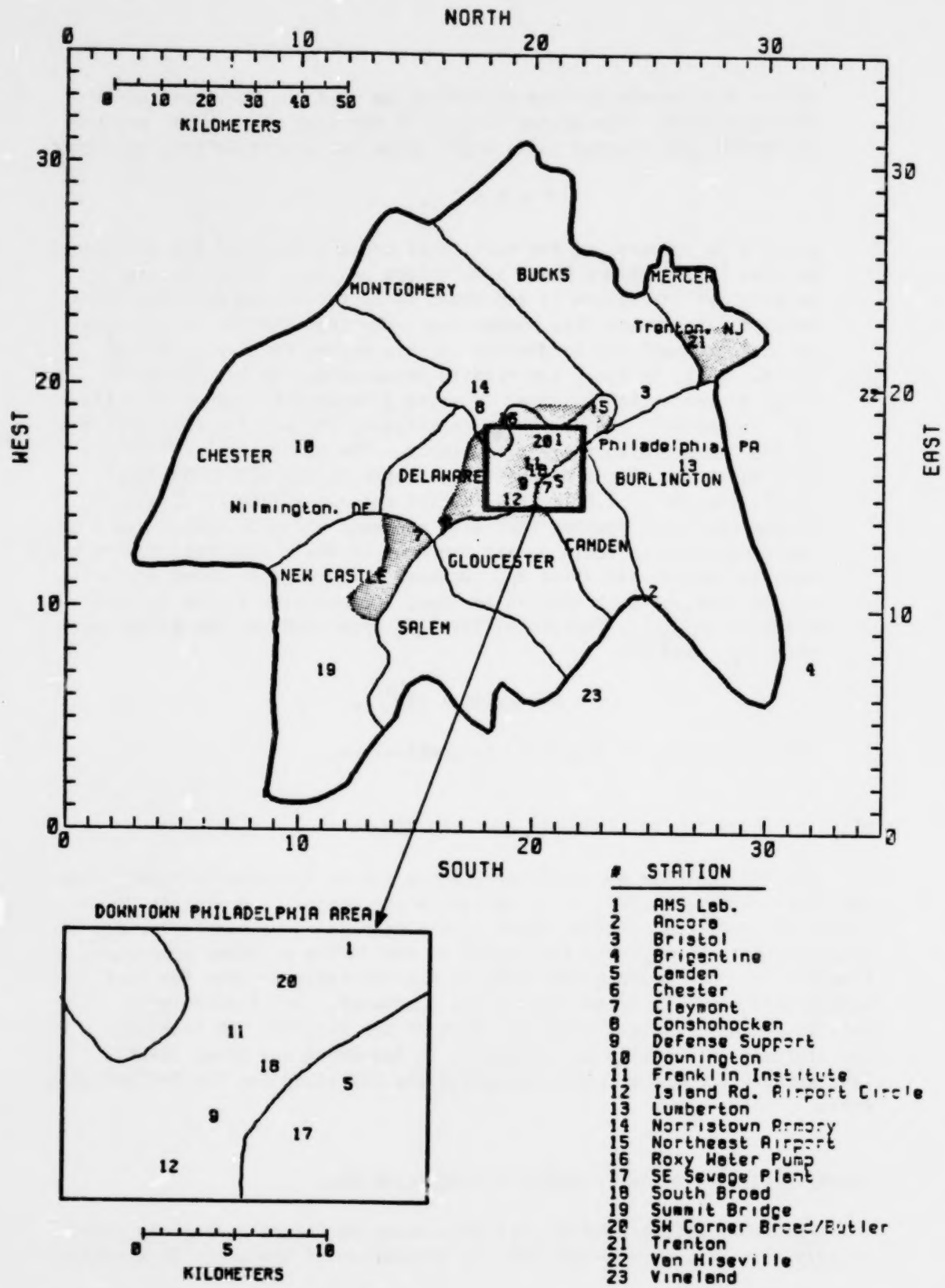


FIGURE 1. Philadelphia airshed modeling region. (Bold outline is emission region; lighter lines are county boundaries.)

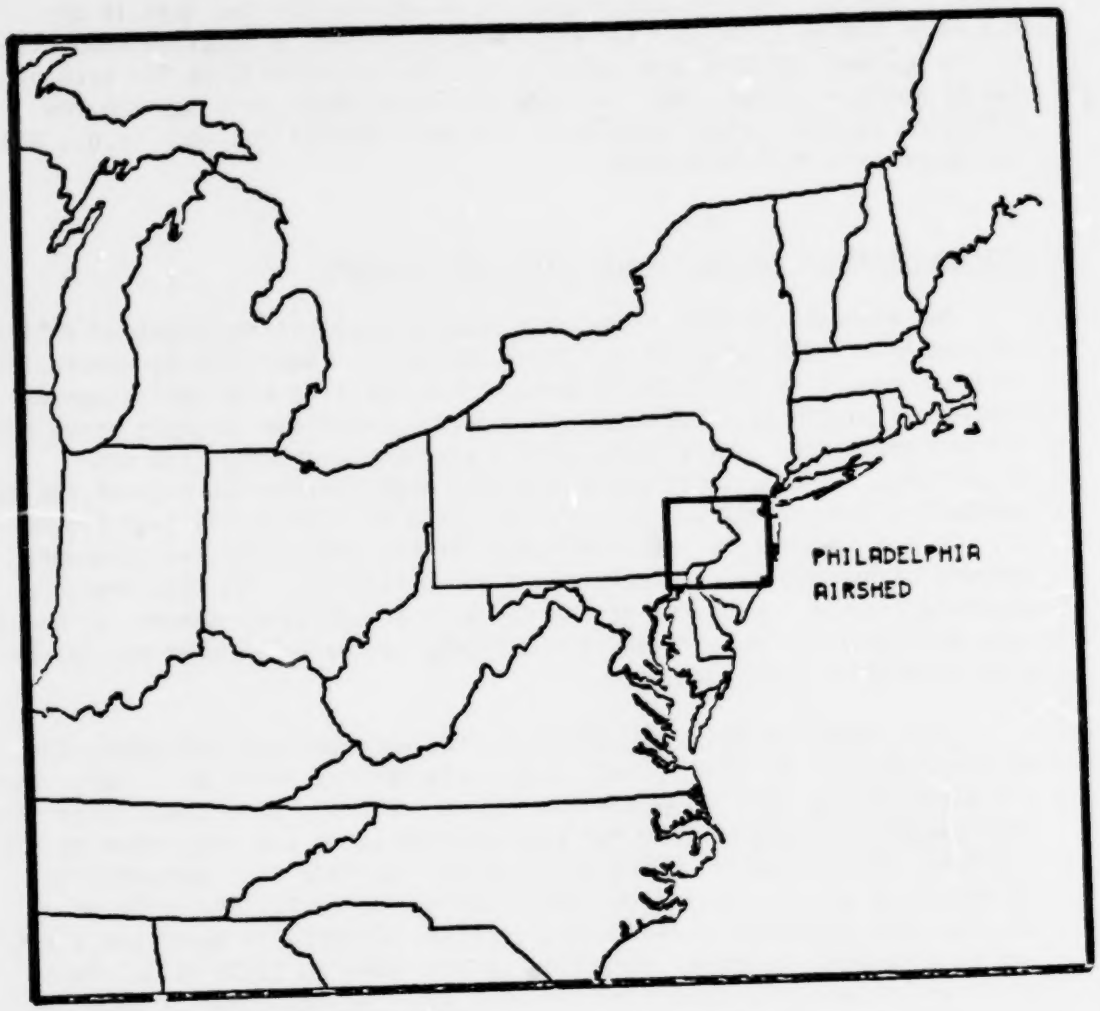


FIGURE 2. Geographical location of the Philadelphia airshed modeling region.

describes the meteorological and air quality conditions associated with the 13 and 19 July 1979 study days, considering, in particular, the general transport characteristics of each day and the resulting pollutant patterns observed over the monitoring network. The maximum observed ozone concentrations and the predicted values for the two days is presented in Tables 1 and 2. Tables 1A and 2A present a detailed comparison of the maximum measured and calculated ozone concentrations for each of the 22 monitoring stations. We note that throughout this section any reference to time refers to time at the beginning of the hour (e.g., 0500 EDT represents 0500-0600 EDT).

Characterization of the 13 July 1979 Ozone Episode

The highest and most widespread ozone concentrations measured during the summer of 1979 occurred on Friday, 13 July. These high concentrations were the result of a buildup of precursors resulting from near-stagnant conditions on the previous day, and generally weak and variable winds prevailing until noon of the 13th, when a stronger southerly flow was established. The synoptic pattern showed high pressure throughout the day dominating the surface and upper-level (2000 m) flow fields (see Figure 3). This high-pressure system was part of the seasonally semipermanent Bermuda high-pressure cell centered east of Florida. The high pressure weakened through the course of the day as a trough (the remnants of Hurricane Bob) over the Ohio Valley moved slowly eastward bringing precipitation to western Pennsylvania.

Light west-northwesterly surface winds were present throughout the region from noon on 12 July until the early-morning hours of 13 July when the winds became calm or very light with a northerly direction. This wind flow pattern was responsible for transporting ozone and precursors to the southeast of the region during this period. Surface wind measurements showed these calm-to-very-light winds during the early-morning hours of 13 July with northerly directions increasing slightly in speed and shifting to a general southerly direction by late morning (1000 EST). This shift in surface wind direction resulted in a recirculation of material that had been transported to the southeast during the previous 24 hours: (1) Influx of ozone and precursor from the southeast; (2) a buildup of regional ozone and precursors from near stagnant conditions on the previous day (12 July); (3) the day's emissions; (4) generally light winds; (5) high region-wide temperatures; and (6) mostly clear skies were the primary conditions leading to high ozone concentrations.

Evidence of this recirculation of ozone and precursor material and the possible existence of a reservoir of ozone aloft from the previous day is shown in the observed ozone concentration data at upwind monitors. For

TABLE 1-A. MAXIMUM PREDICTIONS/OBSERVATIONS FOR 13 JULY 1979 FOR OZONE (pphm)

STATIONS	OBSERVED MAXIMUM CONCENTRATION	PREDICTED MAXIMUM CONCENTRATION	RATIO OF PREDICTED TO OBSERVED CONCENTRATION	PERCENTAGE DIFFERENCE (PR - OB)/OB	HOUR OF OBSERVED MAXIMUM CONCENTRATION	HOUR OF PREDICTED MAXIMUM CONCENTRATION	LAG (HOURS)
AMS LAB	16.00	17.35	1.08	8	1300	1300	0
ANCORA	14.10	13.30	0.94	-5	1400	1300	-1
BRISTOL	13.00	17.95	1.38	38	1600	1500	-1
CAMDEN	16.10	15.47	0.96	-3	1300	1200	-1
CHESTER	18.30	14.56	0.80	-20	1200	1300	1
CLAYMONT	10.00	13.58	1.36	35	1400	1200	-2
CONSHOHOCKEN	20.50	18.46	0.90	-10	1600	1300	-3
DEFENSE SUPP	15.00	14.06	0.94	-6	1300	1200	-1
DOWNINGTON	12.30	12.93	1.05	5	1300	1500	2
FRANKLIN INS	15.00	14.12	0.94	-5	1300	1300	0
ISLAND RD AI	10.00	12.86	1.29	28	1100	1300	2
LUMBERTON	12.50	12.71	1.02	1	1500	1300	-2
NORRISTOWN A	18.30	19.26	1.05	5	1500	1400	-1
ROXY WATER P	20.00	19.32	0.97	-3	1400	1300	-1
SE SEWAGE PL	10.00	15.28	1.53	52	1300	1200	-1
SOUTH BROAD	14.00	14.34	1.02	2	1300	1300	0
SUMMIT BRIDG	8.70	9.79	1.13	12	1000	1200	2
TRENTON	11.30	16.41	1.45	45	1400	1600	2
VAN HISEVILL	9.00	11.32	1.26	25	1200	1600	4

TABLE 1-B. PERFORMANCE MEASURES FOR THE UAM SIMULATION OF THE 13 JULY 1979 EPISODE IN PHILADELPHIA

Performance Attribute	Performance Measure	Values
Accuracy of the airshed peak prediction	Ratio of predicted to measured station peaks	0.940
	Time difference between predicted and measured station peaks	-2 hours
	Station Peaks	
	Predicted	19.3 pphm (Roxy Water)
	Measured	20.5 pphm (Conshohocken)
Station peaks		
Systematic bias	Mean Deviation	
	Normalized	
	Average	-0.086
	Std. dev.	0.180
	Nonnormalized	
	Average	-0.998 pphm
	Std. dev.	2.491 pphm
	Bounds at the 90 percent confidence level	-2.790 and 0.793 pphm
Gross error	Mean absolute deviation	
	Normalized	
	Average	0.148
	Std. dev.	0.130
	Nonnormalized	
	Average	2.021 pphm
	Std. dev.	1.718 pphm

TABLE 1-B (Concluded)

Performance Attribute	Performance Measure	Values
All O_3 Concentrations > 5 pphm		
Systematic bias	Mean deviation	
	Normalized	
	Average	-0.150
	Std. dev.	0.361
	Nonnormalized	
	Average	-1.660 pphm
	Std. dev.	2.885 pphm
Gross error	Mean absolute deviation	
	Normalized	
	Average	0.295
	Std. dev.	0.255
	Nonnormalized	
	Average	2.670 pphm
	Std. dev.	1.981 pphm
Temporal correlation	Temporal correlation coefficients	
	Each station	0.273 to 0.956
	All-station average	0.737
Spatial alignment	Spatial correlation coefficients	
	Each hour	0.041 to 0.735
	All-hour average	0.456

TABLE 2-A. MAXIMUM PREDICTIONS/OBSERVATIONS FOR 19 JULY 1979 FOR OZONE (pphm).

STATIONS	OBSERVED MAXIMUM CONCENTRATION	PREDICTED MAXIMUM CONCENTRATION	RATIO OF PREDICTED TO OBSERVED CONCENTRATION	PERCENTAGE DIFFERENCE (PR - OB)/OB	HOUR OF OBSERVED MAXIMUM CONCENTRATION	HOUR OF PREDICTED MAXIMUM CONCENTRATION	LAG (HOURS)
AMS LAB	13.00	13.39	1.03	3	1200	1500	3
ANCORA	9.70	10.88	1.12	12	1100	1300	2
BRISTOL	11.40	10.22	0.90	-10	1400	1300	-1
BRIGANTINE	5.10	6.80	1.33	33	1400	1200	-2
CAMDEN	13.80	13.31	0.96	-3	1300	1500	2
CHESTER	14.30	10.32	0.72	-27	1500	1400	-1
CLAYMONT	16.00	10.14	0.63	-36	1600	1400	-2
CONSHOHOCKEN	17.00	12.57	0.74	-26	1600	1800	2
DEFENSE SUPP	12.00	13.70	1.14	14	1300	1600	3
DOWNINGTON	15.70	14.21	0.91	-9	1500	1500	0
FRANKLIN INS	6.00	12.71	2.12	111	1100	1600	5
ISLAND RD AI	12.00	13.74	1.14	14	1200	1700	5
LUMBERTON	10.40	9.58	0.92	-7	1100	1200	1
NORRISTOWN A	13.80	13.22	0.96	-4	1600	1500	-1
NORTHEAST AI	10.00	12.61	1.26	26	1400	1400	0
ROXY WATER P	17.00	13.84	0.81	-18	1400	1700	3
SE SEWAGE PL	8.00	13.47	1.68	68	1300	1600	3
SOUTH BROAD	11.00	12.86	1.17	16	1300	1600	3
SUMMIT BRIDG	12.00	8.56	0.71	-28	1400	1200	-2
TRENTON	7.10	8.71	1.23	22	1200	1300	1
VAN HISEVILL	8.30	7.99	0.96	-3	1000	1100	1
VINELAND	10.30	10.53	1.02	2	1300	1400	1

TABLE 2-B. PERFORMANCE MEASURES FOR THE UAM SIMULATION OF THE 19 JULY 1979 EPISODE IN PHILADELPHIA

Performance Attribute	Performance Measure	Values
Accuracy of the airshed peak prediction	Ratio of predicted to measured station peaks	0.836
	Time difference between predicted and measured station peaks	1 hour
	Station Peaks	
	Predicted	14.2 pphm (Downington)
	Measured	17.0 pphm (Roxy Water)
Station peaks		
Systematic bias	Mean deviation	
	Normalized	-0.021
	Average	0.275
	Nonnormalized	
	Average	0.047 pphm
	Std. dev.	3.038 pphm
	Bounds at the 90 percent confidence level	-1.437 and 1.531 pphm
Gross error	Mean absolute deviation	
	Normalized	
	Average	0.205
	Std. dev.	0.179
	Nonnormalized	
	Average	2.293 pphm
	Std. dev.	1.930 pphm

TABLE 2-B (Concluded)

Performance Attribute	Performance Measure	Values
All O_3 concentrations > 5 pphm		
Systematic bias	Mean Deviation	
	Normalized	
	Average	0.005
	Std. dev.	0.398
	Nonnormalized	
	Average	0.024 pphm
	Std. dev.	3.163 pphm
Gross error	Mean absolute deviation	
	Normalized	
	Average	0.288
	Std. dev.	0.273
	Nonnormalized	
	Average	2.400 pphm
	Std. dev.	2.051 pphm
Temporal correlation	Temporal correlation coefficients	
	Each station	-0.914 to 0.970
	All-station average	0.525
Spatial alignment	Spatial correlation coefficients	
	Each hour	-0.421 to 0.643
	All-hour average	0.202

FIGURE 3. Synoptic situation, 0700 EST, July 13, 1979.
(Source: Allard et al., 1981)

the morning of 13 July, stations to the south and east were upwind. Examination of the ozone concentration during the initial onset of mixing is one way of providing information on ozone levels aloft. At 1000 EST, observed ozone concentrations were 8.4 pphm at Brigantine, New Jersey; 9.7 pphm at Lumberton, New Jersey; and 12.3 pphm at Ancora, New Jersey. Another upwind monitor (Vineland, New Jersey) could not provide ozone data for 1000 EST; however, an hour earlier (900 EST) this monitor recorded an ozone concentration of 10.2 pphm. For this time period (onset of mixing), these ozone concentrations were among the highest observed during the summer of 1979. This indicates that a large reservoir of ozone existed aloft and was available for mixing down to the surface.

No upper-air measurements were available in Philadelphia on this day; however, radiosonde data from New York City (JFK Airport) and Washington D.C. (Dulles International Airport) showed very light westerly winds at 2000 m throughout the day.

Because surface wind flow patterns established a southerly direction by late morning, peak ozone concentrations occurred north of the high urban emission source region. The highest ozone concentration recorded on this day was a value of 20.5 pphm at Conshohocken at 1600 EST. The second highest value of 20 pphm occurred earlier in the afternoon at the Roxy Water Pump monitor at 1400 EST. Thirteen monitors recorded ozone concentrations greater than 12 pphm.

Characterization of the 19 July 1979 Ozone Episode

The second-highest peak ozone readings in the Philadelphia Air Quality Control Region (AQCR) during the 1979 summer oxidant data enhancement study occurred on Thursday, 19 July (Allard et al., 1981). On this day, the Philadelphia urban plume was transported to the west of the central city and precursor transport from the New York/New Jersey urban area was the apparent cause of a substantial portion of the ozone concentrations measured in the Philadelphia area.

A broad high-pressure area extending from the midwest through the northeast to Nova Scotia influenced surface wind patterns. The eastern core of this high-pressure area was situated to the north of Philadelphia in the early morning hours, bringing light northerly winds through the airshed. This high-pressure ridge moved eastward throughout the day. As a result, the surface winds veered to an easterly direction around noon and then to a southeasterly flow that persisted the rest of the day. Winds aloft showed a persistent west-southwesterly flow during the entire day. Surface trajectory analysis indicated that air parcels arriving in the urban center of Philadelphia at 1200 EST originated to the northeast in the New Jersey/New York urban area.

The peak ozone concentration recorded on 19 July 1979 was 17.0 pphm at the Roxy Water Pump monitoring station 10 km northeast of central Philadelphia. The same value was also recorded at Conshohocken. An ozone reading of 16.0 pphm was also recorded at Downington, 45 km due west of downtown Philadelphia. Six monitors recorded ozone concentrations equal to or greater than 12 pphm and an additional four monitors recorded ozone concentrations greater than or equal to 10 pphm.

INPUTS USED IN THE URBAN AIRSHED MODEL SIMULATIONS

Detailed descriptions of the meteorological, emissions, and boundary concentration inputs used in the UAM are presented in the appendix to this document. In this section, we summarize some of the inputs used for each of the two modeling days.

The study region used in the Urban Airshed Model simulations was defined during the development of the emission inventory by EPA (1982). The modeling region itself is 12,500 km^2 in area and comprises five counties in New Jersey, five counties in Pennsylvania, and one county in Delaware. The emission grid system used for the emission inventory consists of 502 cells, 5 km on a side. Surrounding the modeling region (Figure 1) is a row of cells representing the boundary cells and containing the boundary conditions (concentrations) used in the UAM simulations. Initial conditions for all species were specified using all available monitoring data in the Philadelphia region and these data are shown in Tables 3 and 4 for 0000 EST on 13 and 19 July.

The physical boundaries used in the 13 July simulation are presented in Figure 4. Because of the stagnation characteristics of this episode, much of the large airshed region was "blocked off" and not included in the simulation. No cells containing major emission sources were excluded by this procedure. Estimated background values for all species for 13 July were designated for all boundaries except the Southeast boundary (Table 5). Concentrations of NO, NO_2, CO, and hydrocarbons were specified on the basis of work by Killus (1982) to reflect concentrations of a typical urban atmosphere. Because an urban plume from Philadelphia was transported to the east late on 12 July and then recirculated back by a southeasterly flow on the 13 July, there is a different set of concentrations for the Southeast boundary grid cells below the mixing height (Table 6). The concentrations were made to duplicate the inflow of aged air parcels from the previous day's emissions.

Because of wind flow through the airshed on 19 July and the need to limit simulation costs, certain unnecessary grid cells were eliminated.

TABLE 3. INITIAL CONDITIONS FOR 13 JULY 1979 (CONCENTRATIONS IN PPM)

Station	Easting (m)	Northing (m)	NO	NO_2	CO	O_3	RHC
AMS Lab.	491600	4428500	0.005	0.075	1.5	0.035	1.05
Ancora	511800	4392400	--	--	--	0.051	--
Brigantine	546000	4377506	--	--	--	0.037	--
Bristol	511000	4440000	--	--	--	0.000	--
Camden	491700	4419000	0.022	0.105	2.4	0.004	--
Chester	469000	4410000	--	0.030	--	0.058	2.10
Claymont	461500	4406400	--	0.045	--	--	--
Conshohocken	474500	4435600	--	--	--	0.000	--
Defense Support	483800	4418300	--	--	--	0.020	--
Downington	436000	4426000	0.002	0.012	0.2	0.073	0.00
Franklin Inst.	485200	4422800	0.010	0.065	--	0.035	--
Island Rd. Airp. Cir.	480300	4414800	--	--	--	0.010	--
Lumberton	518000	4423000	0.006	0.031	1.2	0.010	0.20
Norristown Armory	473500	4440000	--	0.075	--	0.000	0.39
Northeast Airp.	499000	4436000	0.035	0.060	--	0.000	--
Roxy Water Pump	479500	4433100	--	--	--	0.045	--
SE Sewage Plant	487200	4417300	--	--	--	0.010	--
South Broad	486100	4421600	0.020	0.080	3.5	0.035	0.30
Summit Bridge	441000	4376000	0.000	0.003	0.2	0.046	0.05
SW Corner Broad/Butler	487000	4428000	--	--	--	0.035	--
Trenton	520000	4452000	--	--	--	0.009	--
Van Hiseville	559000	4439500	0.001	0.006	0.2	0.005	--
Vineland	498200	4371200	--	0.024	--	0.054	--

RHC Component	Carbon-Bond Fraction (% as Carbon)
PAR	74.0
OLE	2.8
ETH	4.1
ARO	13.2
CARB	5.9

TABLE 4. INITIAL CONDITIONS FOR 19 JULY 1979 (CONCENTRATIONS IN PPM)

Station	Easting (m)	Northing (m)	NO	NO_2	CO	O_3	RHC
AMS Lab.	491600	4428500	0.000	0.025	0.5	0.015	0.35
Ancora	511800	4392400	--	--	--	0.015	--
Brigantine	546000	4337506	--	--	--	0.017	--
Bristol	511000	4440000	--	0.039	--	0.012	--
Camden	491700	4419000	0.011	0.051	2.5	0.004	--
Chester	469000	4410000	--	0.024	--	0.026	0.95
Claymont	461500	4406400	--	0.045	--	0.020	--
Conshohocken	474500	4435600	--	--	--	0.000	--
Defense Support	483800	4418300	--	--	--	0.000	--
Downington	436000	4426000	0.006	0.015	0.2	0.024	0.05
Franklin Inst.	485200	4422800	0.030	0.050	0.5	0.010	--
Island Rd. Airp. Cir.	480300	4414800	--	--	--	0.015	--
Lumberton	518000	4423000	0.000	0.028	0.0	0.008	0.40
Norristown Armory	473500	4440000	--	--	--	0.030	0.29
Northeast Airp.	499000	4436000	0.000	0.015	--	--	--
Roxy Water Pump	479500	4433100	--	--	--	0.010	--
SE Sewage Plant	487200	4417300	--	--	--	0.005	--
South Broad	486100	4421600	0.020	0.045	1.5	0.010	0.25
Summit Bridge	441000	4376000	0.000	0.009	0.2	0.009	0.10
SW Corner Broad/Butler	487000	4418000	--	--	--	--	--
Trenton	520000	4452000	--	--	--	0.002	--
Van Hiseville	559000	4439500	0.000	0.006	0.2	0.021	--
Vineland	498200	4371200	--	0.025	--	0.010	--

RHC Component	Carbon-Bond Fraction (% as Carbon)
PAR	74.0
OLE	2.8
ETH	4.1
ARO	13.2
CARB	5.9

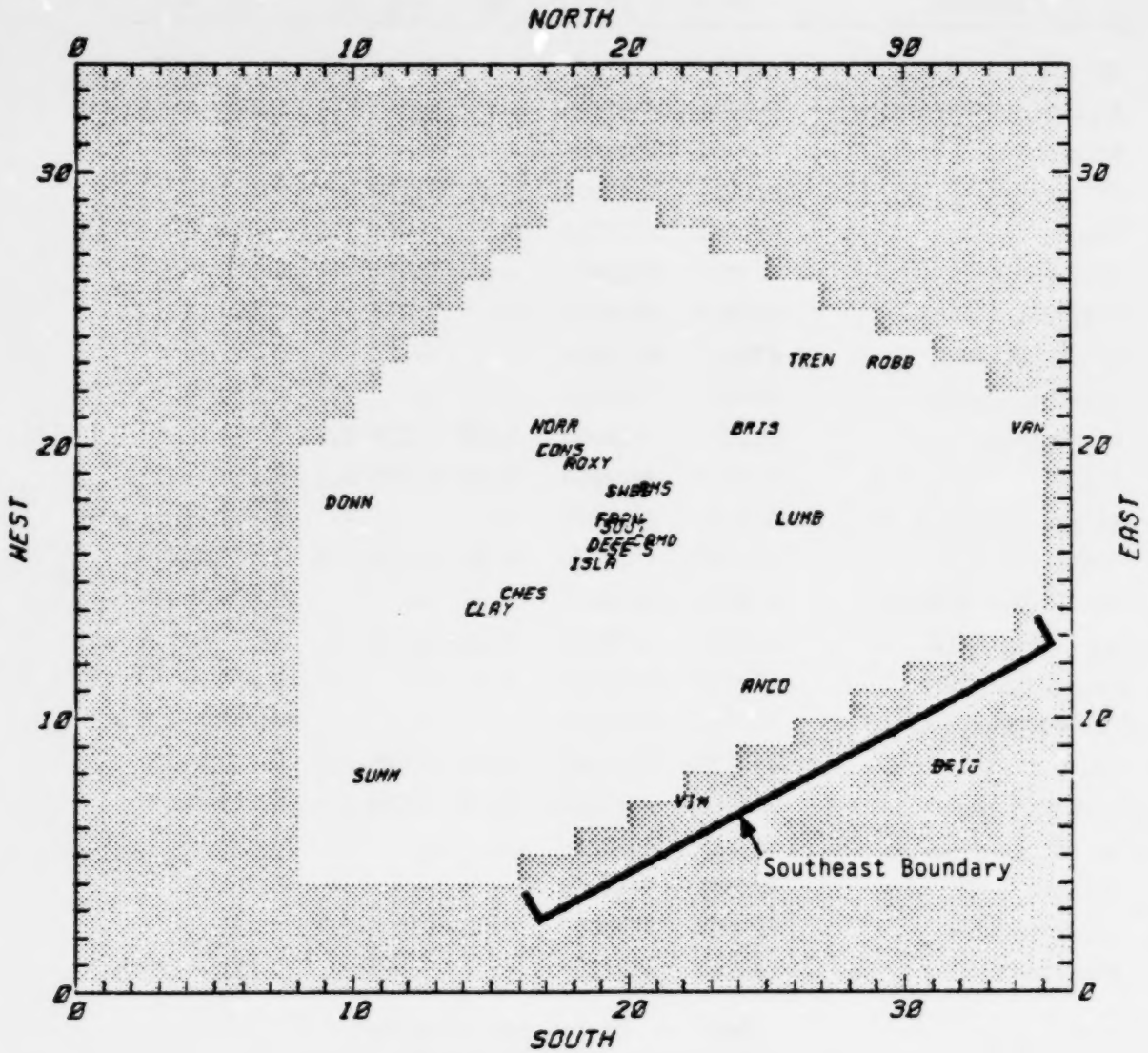


FIGURE 4. Physical boundaries used in the 13 July 1979 Airshed Model simulation (shaded area is not included in the simulation).

TABLE 5. BACKGROUND CONCENTRATION VALUES FOR 13 JULY AT THE TOP OF THE MODELING REGION--AS INITIAL CONCENTRATIONS ABOVE THE MIXING HEIGHT, AND FOR ALL LEVELS OF ALL BOUNDARIES EXCEPT THE LEVELS BELOW THE MIXING HEIGHT ON THE SOUTHEAST BOUNDARY

Species	Concentration (ppm)
NO	0.001
NO_2	0.002
O_3	0.08
CO	0.2
ETH	0.001
OLE	0.0004
PAR	0.040
CARB	0.010
ARO	0.0008
PAN	0.000025
BZA	0.00001

TABLE 6. SOUTHEAST BOUNDARY CONDITIONS FOR CELLS BELOW THE MIXING HEIGHT FOR THE SIMULATION OF 13 JULY 1979 (CONCENTRATIONS IN PPM)

Time interval	NO	NO_2	O_3	PAR	OLE	ETH	ARO	CARB	PAN
0000-0100	0.001	0.009	0.053	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0100-0200	0.001	0.009	0.041	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0200-0300	0.001	0.009	0.037	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0300-0400	0.001	0.009	0.036	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0400-0500	0.001	0.009	0.028	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0500-0600	0.001	0.009	0.010	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0600-0700	0.001	0.009	0.021	0.1041	0.00105	0.0026	0.0021	0.0261	0.0040
0700-0800	0.001	0.007	0.035	0.0983	0.00065	0.0022	0.0017	0.0259	0.0044
0800-0900	0.001	0.004	0.072	0.0904	0.00040	0.0018	0.0012	0.0244	0.0054
0900-1000	0.001	0.002	0.102	0.0825	0.00040	0.0015	0.0008	0.0218	0.0062
1000-1100	0.001	0.002	0.111	0.0758	0.00040	0.0012	0.0008	0.0188	0.0062
1100-1200	0.001	0.002	0.121	0.0698	0.00040	0.0010	0.0008	0.0157	0.0058
1200-1300	0.001	0.002	0.139	0.0644	0.00040	0.0010	0.0008	0.0129	0.0052
1300-1400	0.001	0.002	0.113	0.0596	0.00040	0.0010	0.0008	0.0107	0.0047
1400-1500	0.001	0.002	0.105	0.0546	0.00040	0.0010	0.0008	0.0100	0.0040
1500-1600	0.001	0.002	0.093	0.0525	0.00040	0.0010	0.0008	0.0100	0.0037
1600-1700	0.001	0.002	0.069	0.0506	0.00040	0.0010	0.0008	0.0100	0.0032
1700-1800	0.001	0.002	0.068	0.0506	0.00040	0.0010	0.0008	0.0100	0.0032

TABLE 6. CONCLUDED

Time interval	NO	NO_2	O_3	PAR	OLE	ETH	ARO	CARB	PAN
1800-1900	0.001	0.002	0.058	0.0506	0.0004	0.001	0.0008	0.010	0.0032
1900-2000	0.001	0.002	0.065	0.0506	0.0004	0.001	0.0008	0.010	0.0032
2000-2100	0.001	0.002	0.059	0.0506	0.0004	0.001	0.0008	0.010	0.0032
2100-2200	0.001	0.002	0.056	0.0506	0.0004	0.001	0.0008	0.010	0.0032
2200-2300	0.001	0.002	0.051	0.0506	0.0004	0.001	0.0008	0.010	0.0032
2300-2400	0.001	0.002	0.050	0.0506	0.0004	0.001	0.0008	0.010	0.0032

The physical boundaries used in the simulation are shown in Figure 5. Background values were designated for all boundaries except the East and Northeast boundaries. Estimates of boundary conditions for the East and Northeast boundaries below the mixing height are presented in Table 7. Observed NO and NO_2 for the 0500-0600 EST were used as input boundary values for 0000-0600. Since hydrocarbons were not measured at the Van Hiseville monitor, estimates of the influx of total reactive hydrocarbons across the Northeast and East boundaries below the mixing height were specified by multiplying the hourly NO_x concentrations at the Van Hiseville Monitor by the Philadelphia surface emission inventory hydrocarbon/NO_x ratio of 6.

Mixing height profiles for 13 July were estimated using temperature soundings of JFK and Dulles airports since no soundings were available for Philadelphia on this day. Mixing heights for 13 July are shown in Table 8 and Figure 6. Mixing height profiles were developed for 19 July using available radiosonde observations and sodar data for the Philadelphia area. Mixing heights for 19 July are shown in Table 9 and Figure 7.

Three-dimensional wind fields for 13 July and 19 July were generated from station measurements and aloft winds obtained from radiosonde data. Wind direction on the morning of 13 July was very light and from the north. Around 1000 EST, however, a shift occurred and winds with higher speeds came from the southeast for the rest of the day. Winds on the morning of 19 July were predominantly from the north. Throughout the day a 180° shift occurred; at noon the wind direction was predominantly from the east; during the evening it came from the south-southeast. The gridded, smoothed surface vectors for selected hours are presented in Figure 8 for 13 July and in Figure 9 for 19 July.

Except for the ozone concentration, the estimated background concentrations above the mixing height are the same for both days. On the basis of examination of upwind monitoring data at the time of mixing, the value specified for ozone was reduced to 0.06 ppm. Estimated background concentrations are listed in Table 10. The gridded and elevated point source emission inventory was prepared for EPA in 1981 by Engineering Science, Inc. (EPA, 1982). Daily emission values for total NO_x and total hydrocarbon are presented in Table 11.

INPUTS USED IN THE SYSTEMS APPLICATIONS TRAJECTORY MODEL SIMULATIONS

The meteorological and emissions files used in the Systems Applications Trajectory Model are the same as those used by the UAM. By running the Systems Applications Trajectory Model in a backward mode, a path to the maximum ozone observed can be determined for the day of interest.

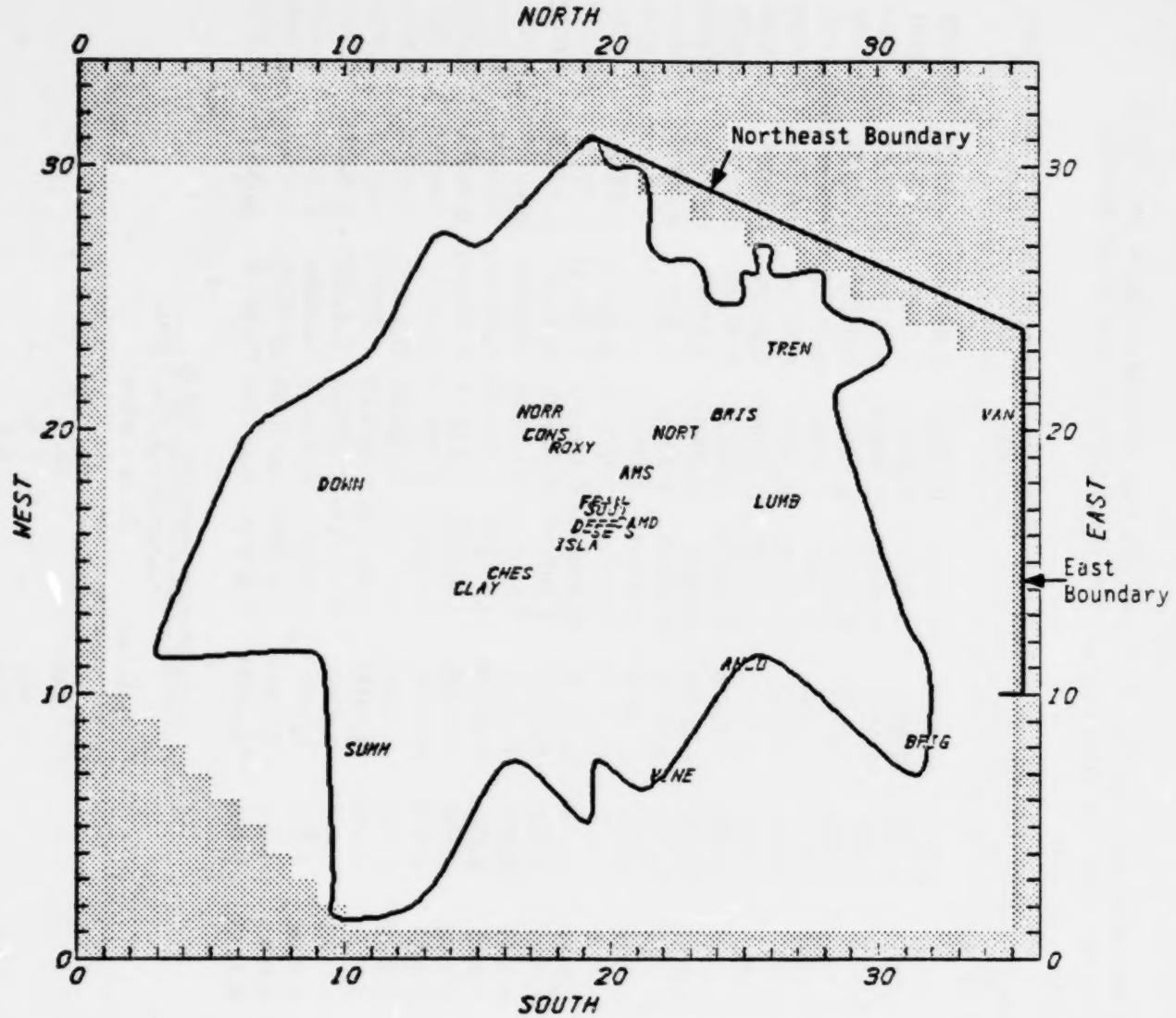


FIGURE 5. Boundary specifications for 19 July 1979 simulation. (Bold line is emissions region.)

TABLE 7. BOUNDARY CONDITIONS USED FOR THE NORTHEAST AND EAST BOUNDARIES BELOW THE MIXING HEIGHT ESTIMATED FROM DATA COLLECTED AT THE VAN HISEVILLE, NEW JERSEY MONITOR (concentrations in ppm)

Hour (EST)	NO	NO_2	O_3	PAR	OLE	ETH	ARO	CARB	PAN
0000-0100	0.044	0.036	0.018	0.3552	0.00672	0.00985	0.01056	0.02832	0.0002
0100-0200	0.044	0.036	0.009	0.3552	0.00672	0.00985	0.01056	0.02832	0.0001
0200-0300	0.044	0.036	0.000	0.3552	0.00672	0.00985	0.01056	0.02832	0.0000
0300-0400	0.044	0.036	0.000	0.3552	0.00672	0.00985	0.01056	0.02832	0.0000
0400-0500	0.044	0.036	0.000	0.3552	0.00672	0.00985	0.01056	0.02832	0.0000
0500-0600	0.044	0.036	0.000	0.3552	0.00672	0.00985	0.01056	0.02832	0.0000
0600-0700	0.047	0.041	0.000	0.39072	0.00739	0.010825	0.01162	0.03115	0.0000
0700-0800	0.043	0.0494	0.004	0.40996	0.007755	0.01135	0.01218	0.03269	0.0004
0800-0900	0.026	0.0478	0.015	0.32782	0.0062	0.00908	0.00975	0.02614	0.0008
0900-1000	0.009	0.0273	0.051	0.16132	0.00305	0.00447	0.0048	0.01286	0.0013
1000-1100	0.001	0.0099	0.083	0.04839	0.000915	0.00134	0.00143	0.00386	0.0019
1100-1200	0.000	0.0058	0.078	0.02575	0.000487	0.000716	0.000767	0.00205	0.0018
1200-1300	0.000	0.0054	0.075	0.02397	0.0004535	0.000665	0.000717	0.00191	0.0014
1300-1400	0.000	0.0072	0.072	0.03196	0.000605	0.000885	0.00095	0.00255	0.0012
1400-1500	0.000	0.0047	0.072	0.02087	0.0003945	0.000578	0.00062	0.00166	0.0007
1500-1600	0.000	0.0035	0.062	0.01554	0.000294	0.0004305	0.000462	0.00124	0.0005
1600-1700	0.000	0.0043	0.059	0.01909	0.000361	0.000529	0.000568	0.00152	0.0003
1700-1800	0.000	0.0053	0.052	0.0235	0.000445	0.000652	0.0007	0.001876	0.0003
1800-1900	0.000	0.0072	0.044	0.03197	0.000605	0.000885	0.00095	0.00255	0.0002
1900-2000	0.000	0.0071	0.036	0.03152	0.0005965	0.000875	0.000937	0.00251	0.0001
2000-2100	0.000	0.0041	0.020	0.0182	0.0003445	0.000505	0.000542	0.00145	0.0001
2100-2200	0.002	0.0030	0.010	0.0222	0.00042	0.000615	0.00066	0.00177	0.0000
2200-2300	0.005	0.0060	0.000	0.04884	0.000925	0.001355	0.00145	0.00389	0.0000
2300-2400	0.008	0.0030	0.001	0.04884	0.000925	0.001355	0.00145	0.00389	0.0000

Philadelphia Inventory Split

Species	Carbon-Bond Fraction (% as Carbon)
PAR	74.
OLE	2.8
ETH	4.1
ARO	13.2
CARB	5.9

TABLE 8. URBAN AND RURAL MIXING HEIGHT VALUES USED IN THE DIFFBREAK FILE FOR 13 JULY 1979

Time (EST)	Urban (m)	Rural (m)
0000	250	100
0030	250	100
0100	250	100
0130	250	100
0200	250	100
0230	250	100
0300	250	100
0330	250	100
0400	250	100
0430	250	100
0500	250	100
0530	250	100
0600	250	100
0630	270	135
0700	295	150
0730	375	250
0800	450	350
0830	680	620
0900	925	925
0930	1160	1160
1000	1200	1200
1030	1330	1330
1100	1480	1480
1130	1480	1480
1200	1480	1480
1230	1500	1500
1300	1530	1530
1330	1530	1530
1400	1530	1530
1430	1475	1475
1500	1420	1420
1530	1365	1365
1600	1310	1310
1630	1220	1220
1700	1130	1130
1730	1035	1035
1800	950	950
1830	855	730
1900	770	525
1930	675	320
2000	590	100
2030	500	100
2100	410	100
2130	370	100
2200	330	100
2230	290	100
2300	250	100
2330	250	100
2400	250	100

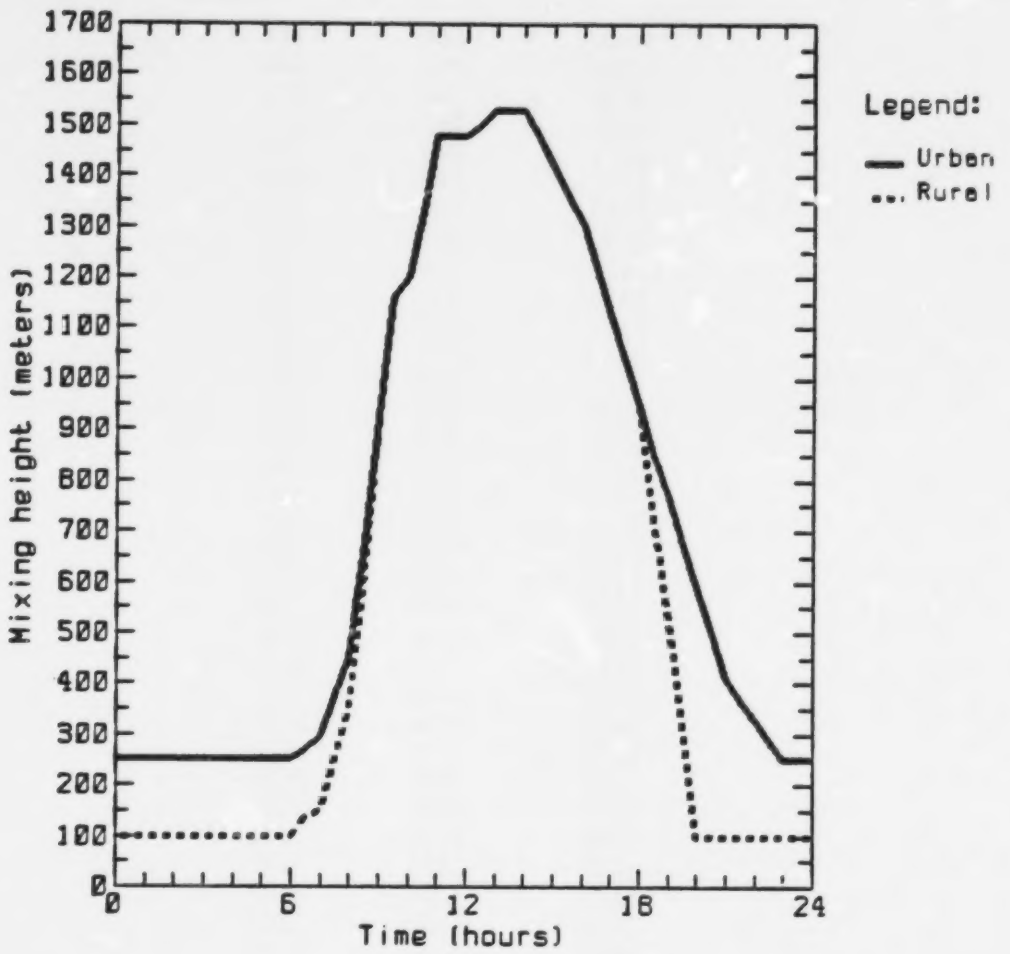


FIGURE 6. Mixing height profile for urban and rural cells for the 13 July 1979 simulation.

TABLE 9. URBAN AND RURAL MIXING HEIGHT VALUES USED IN THE DIFFBREAK FILE FOR 19 JULY 1979

Time (EST)	Urban (m)	Rural (m)
0000	190	100
0030	190	100
0100	190	100
0130	190	100
0200	190	100
0230	190	100
0300	190	100
0330	190	100
0400	190	100
0430	190	100
0500	190	100
0530	190	100
0600	190	100
0630	190	100
0700	190	100
0730	240	260
0800	350	440
0830	460	490
0900	600	540
0930	740	560
1000	890	580
1030	1060	630
1100	1240	880
1130	1420	1320
1200	1530	1430
1230	1530	1430
1300	1480	1380
1330	1410	1310
1400	1340	1240
1430	1270	1170
1500	1200	1100
1530	1120	1020
1600	1020	920
1630	940	840
1700	850	750
1730	750	480
1800	660	160
1830	570	100
1900	480	100
1930	410	100
2000	340	100
2030	300	100
2100	250	100
2130	250	100
2200	250	100
2230	250	100
2300	250	100
2330	250	100
2400	250	100

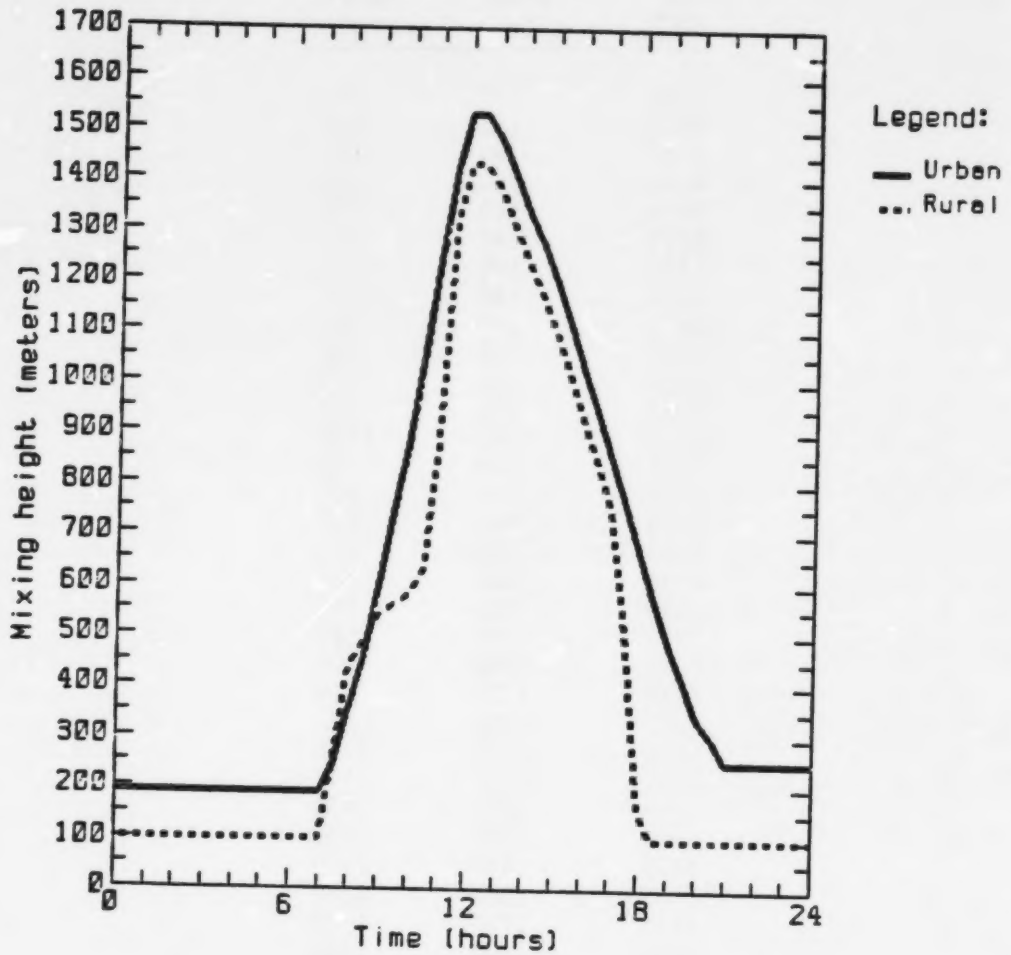
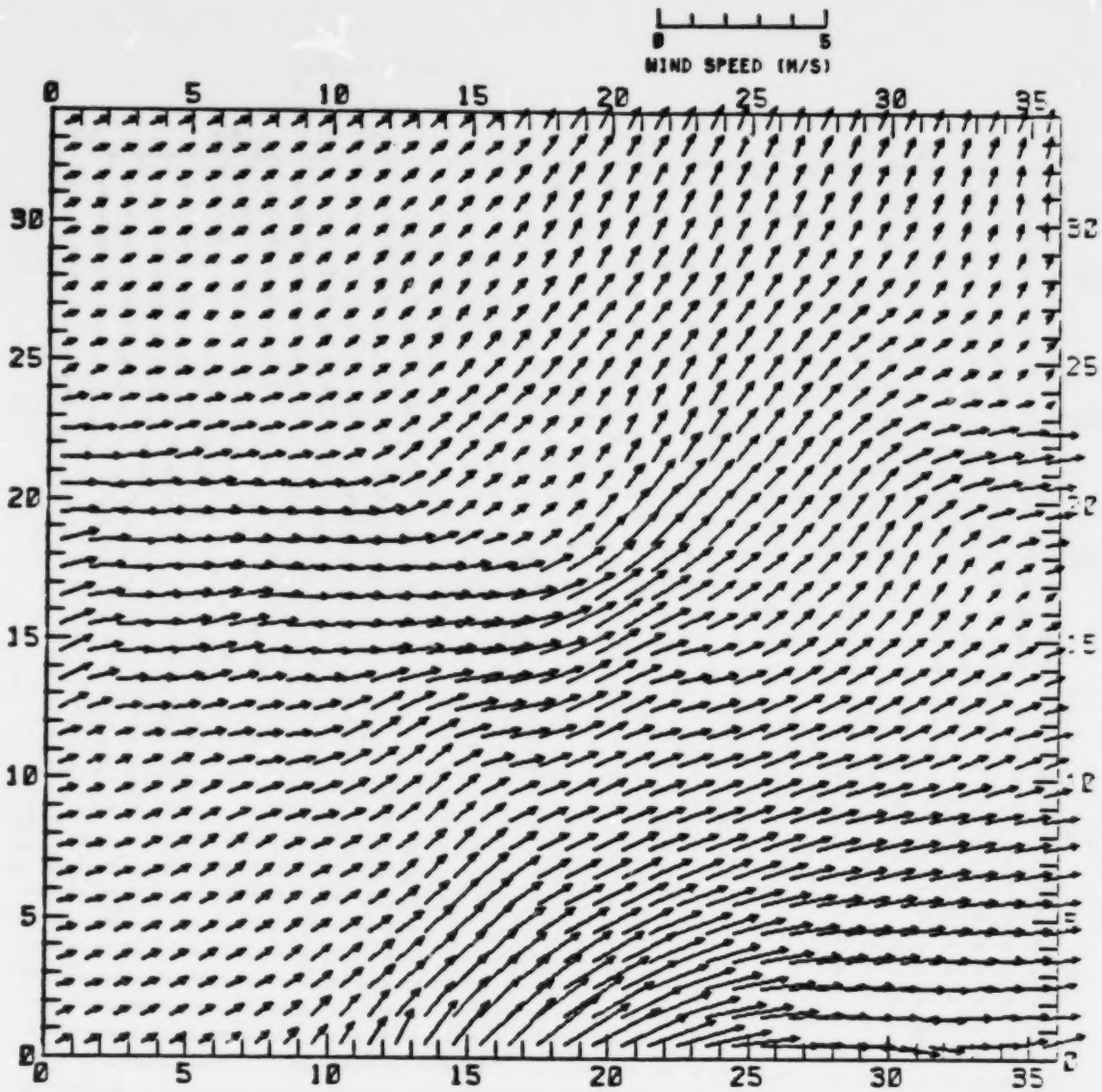
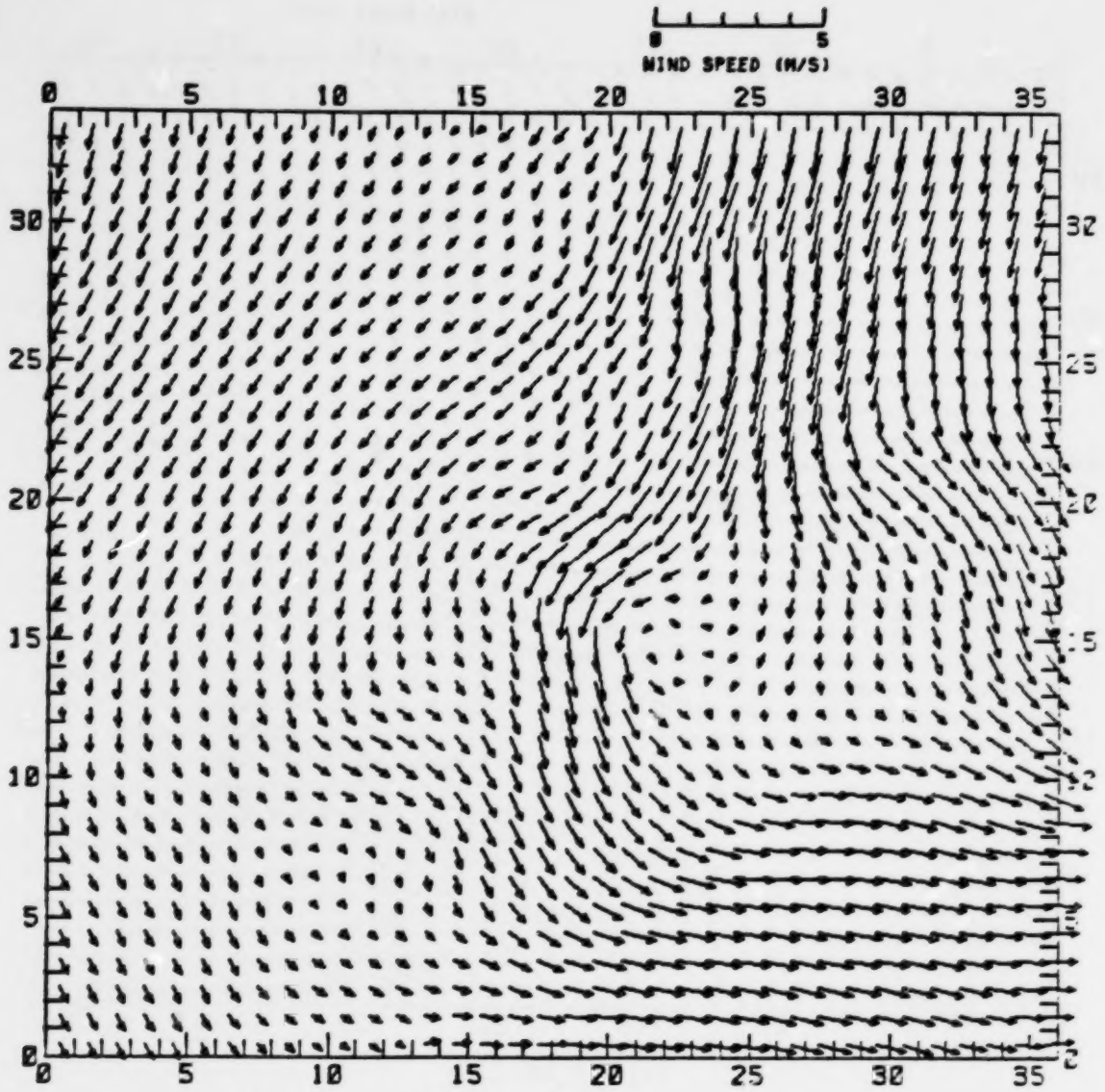


FIGURE 7. Mixing height profiles for urban and rural cells on 19 July 1979.



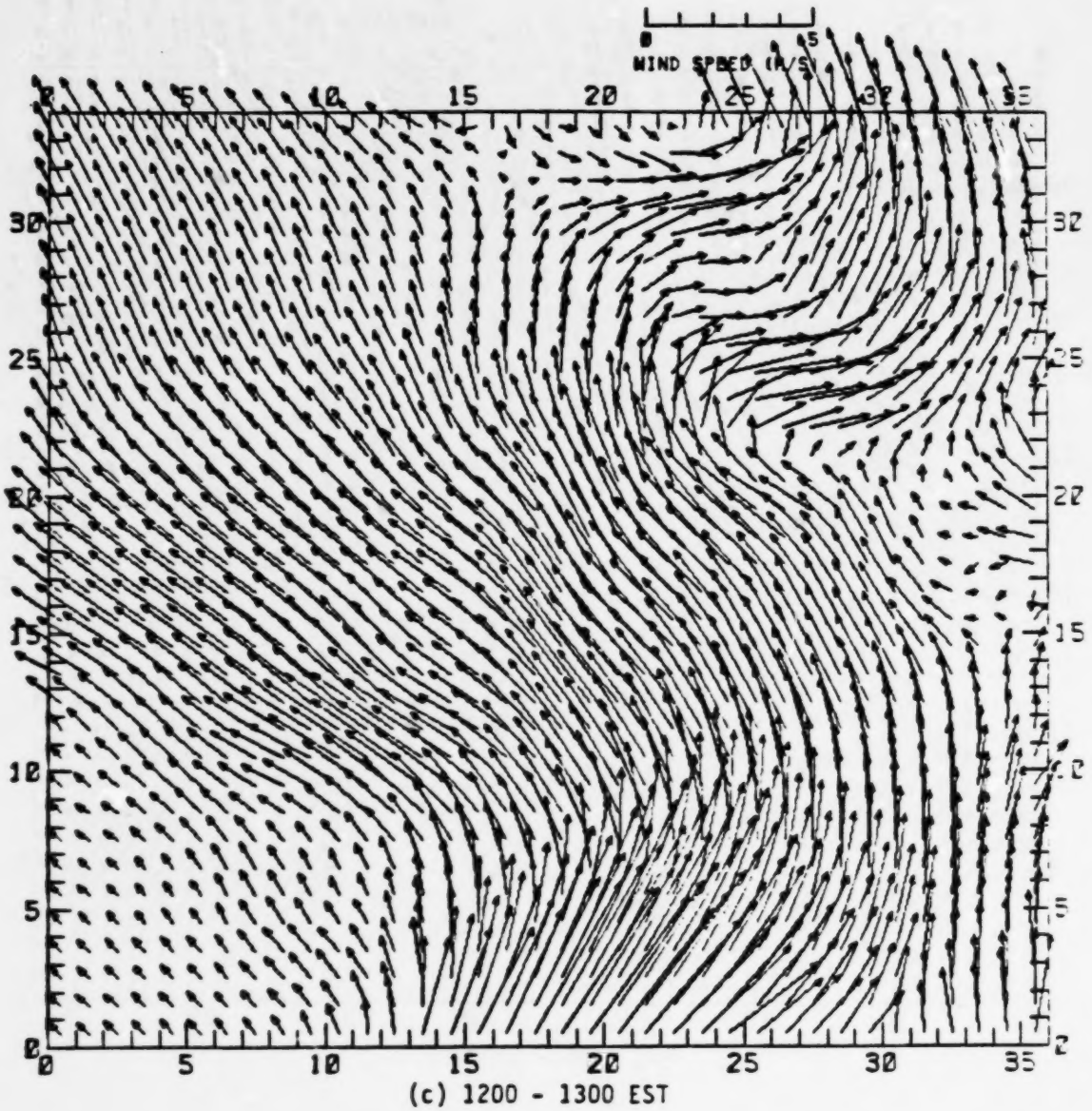
(a) 0 - 100 EST

FIGURE 8. Airshed model surface winds for 13 July 1979.



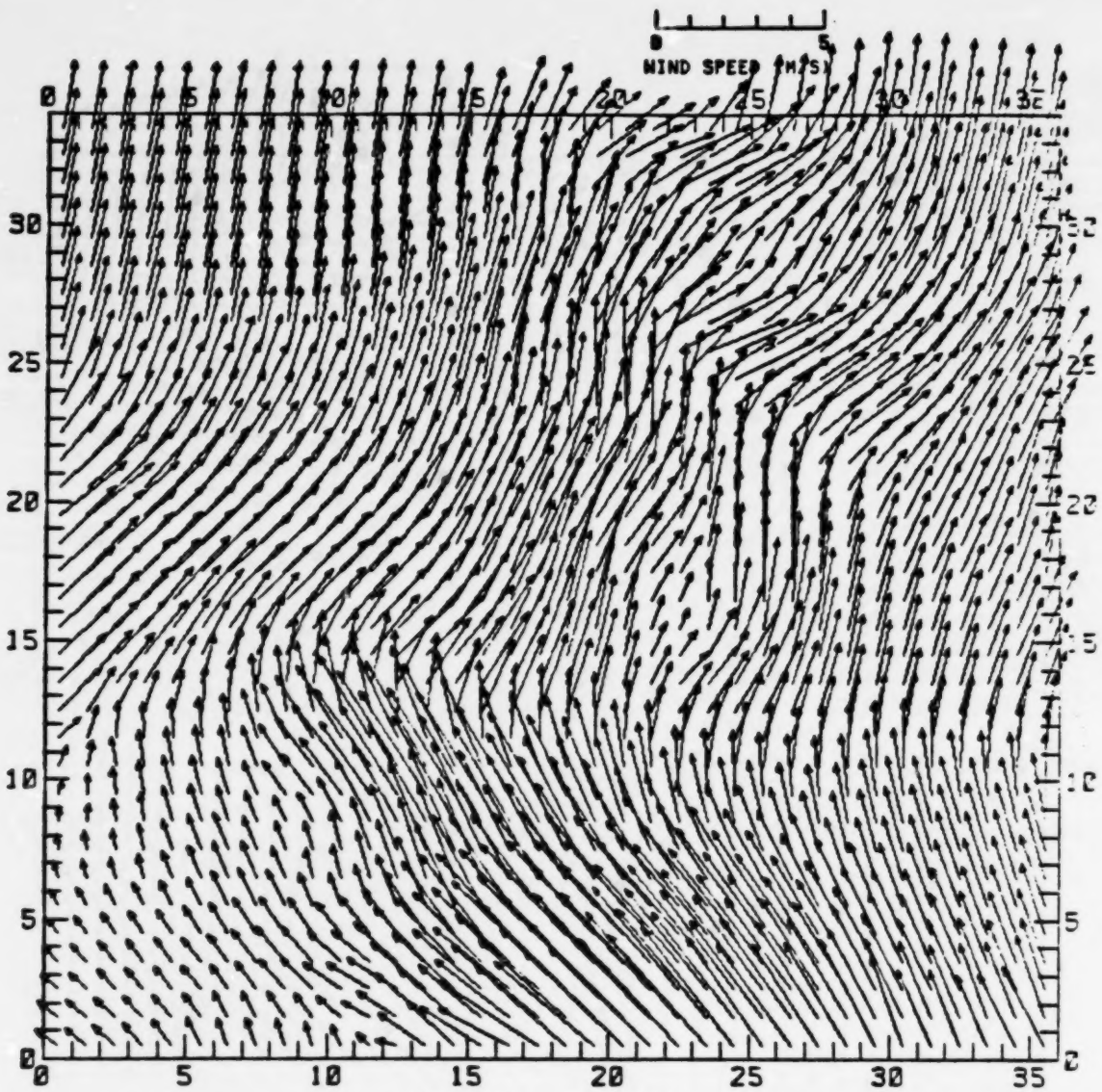
(b) 600 - 700 EST

FIGURE 8 (continued)



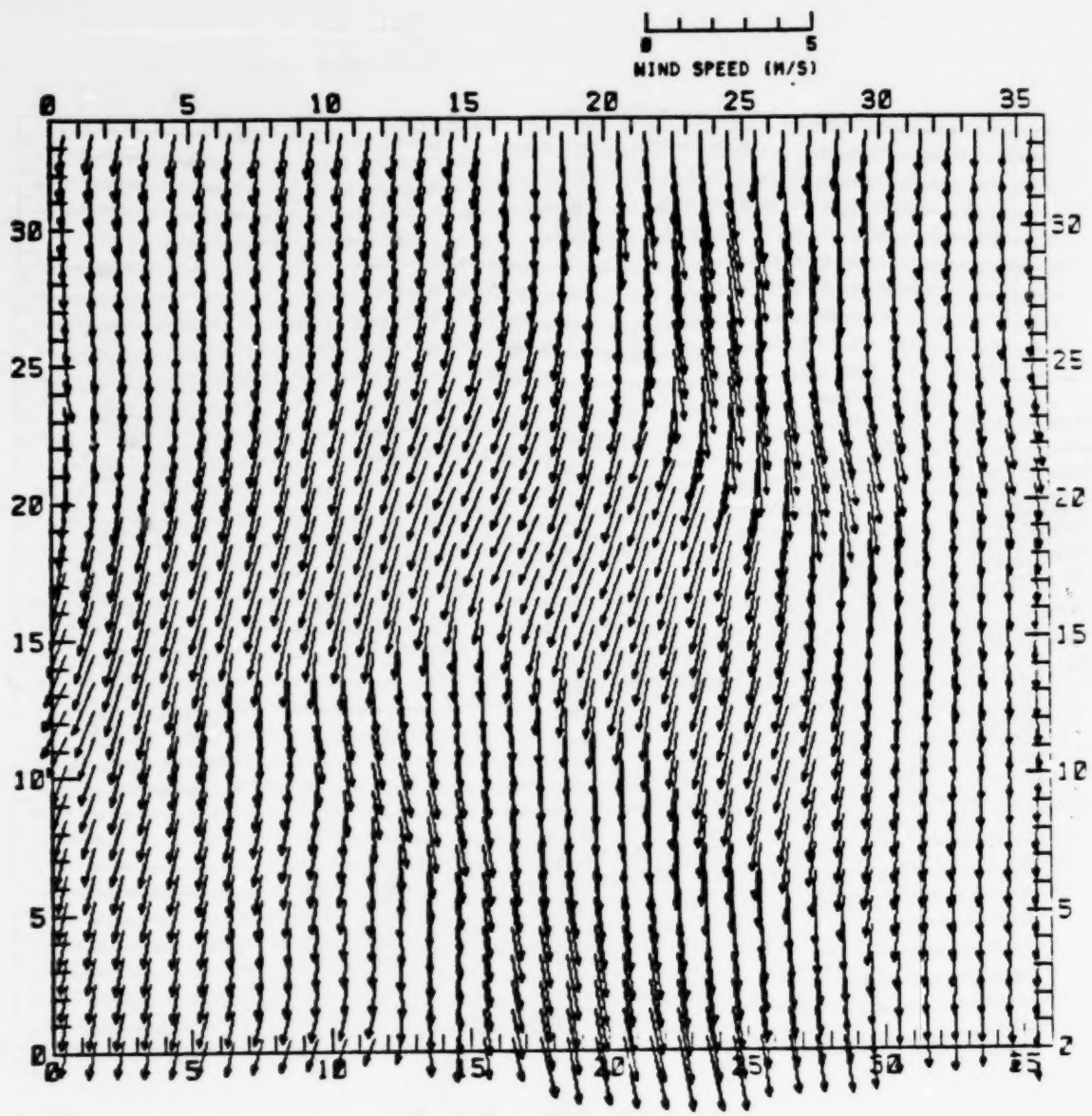
(c) 1200 - 1300 EST

FIGURE 8 (continued)



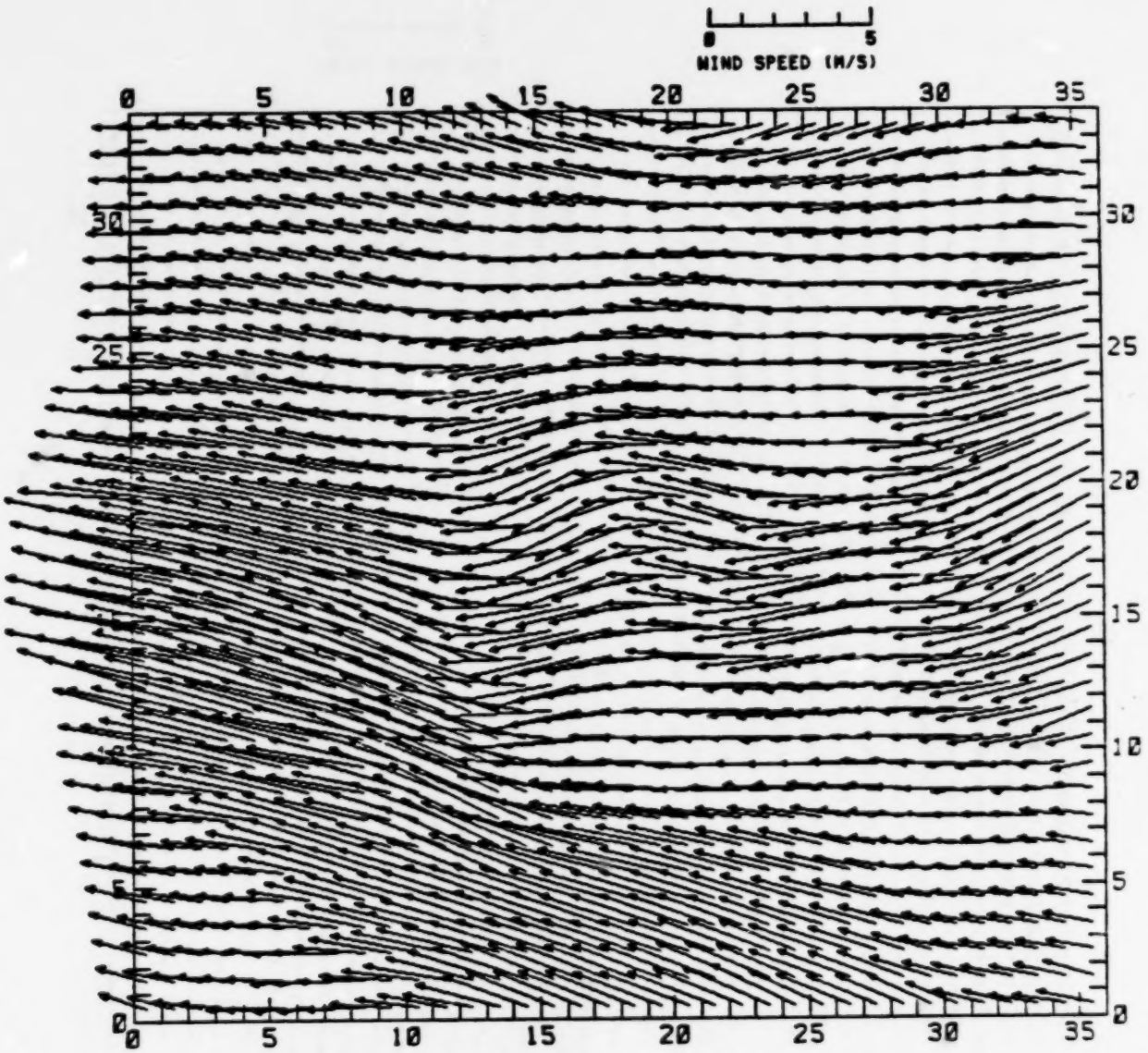
(d) 1800 - 1900 EST

FIGURE 8 (concluded)



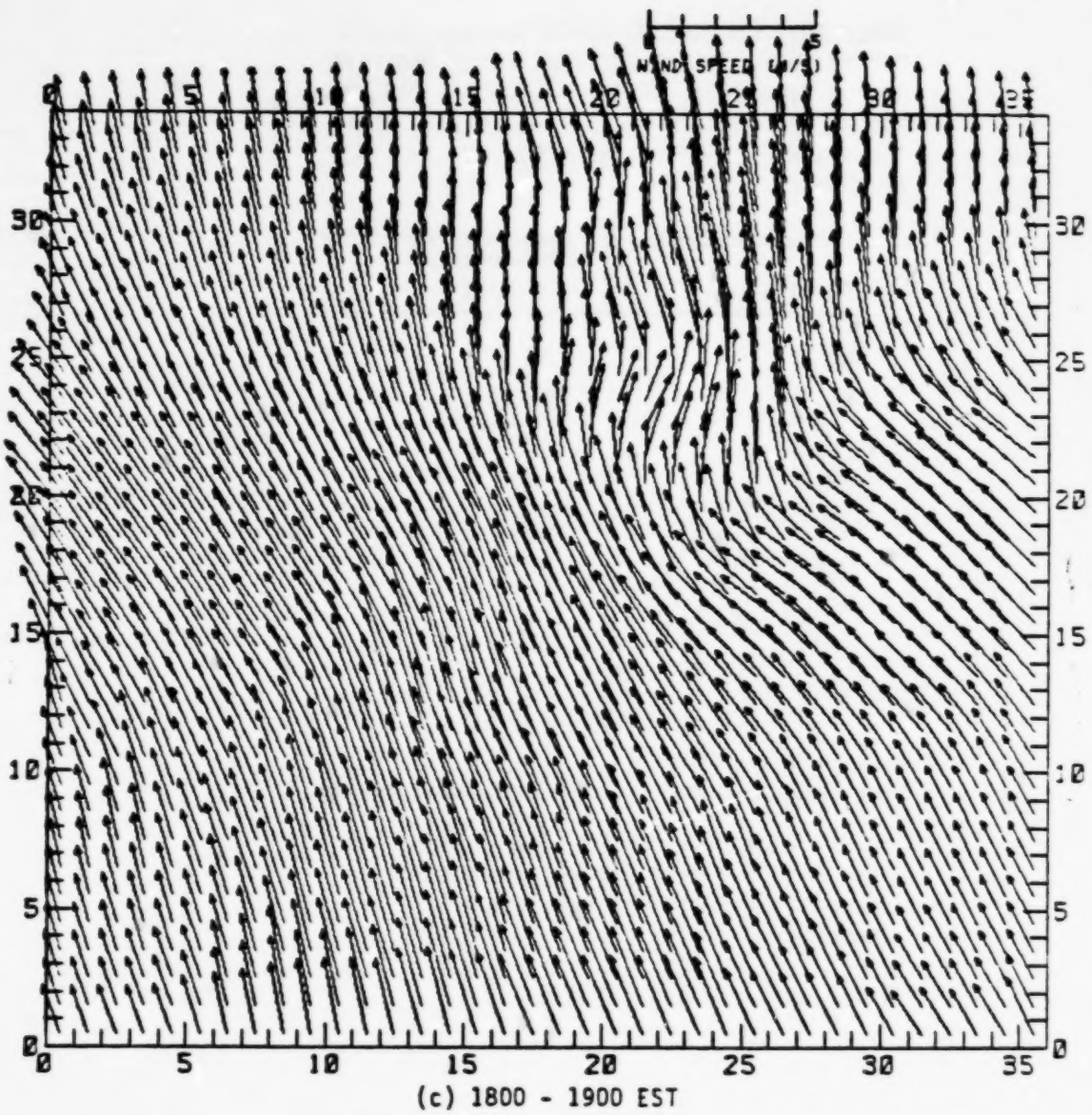
(a) 400 - 500 EST

FIGURE 9. Airshed model surface winds for 19 July 1979.



(b) 1200 - 1300 EST

FIGURE 9 (continued).



(c) 1800 - 1900 EST

FIGURE 9 (concluded).

TABLE 10. BACKGROUND CONCENTRATION VALUES FOR 19 JULY USED AT THE TOP OF THE MODELING REGION (TOPCONC), AS INITIAL CONDITIONS, AND FOR ALL BOUNDARIES EXCEPT THE LEVELS BELOW THE MIXING HEIGHT ON THE NORTHEAST AND EAST BOUNDARIES

Species	Concentration (ppm)
NO	0.001
NO_2	0.002
O_3	0.06*
CO	0.2
ETH	0.001
OLE	0.0004
PAR	0.040
CARB	0.010
ARO	0.0008
PAN	0.000025
BZA	0.00001

* A value of 0.05 ppm was used below the mixing height for all boundaries except the Northeast and East boundaries.

TABLE 11. TOTAL DAILY EMISSIONS BY SOURCE TYPE (mole) IN THE 1979 PHILADELPHIA INVENTORY

Source	NO	NO_2	ETH	OLE	PAR	CARB	ARO
Elevated Point	5,738,955	257,086	12,144	7,792	901,823	570,765	139,960
Minor Point	2,041,679	114,837	385,284	183,632	15,846,729	818,880	510,799
Area Source	2,705,097	207,808	295,258	194,471	26,841,693	1,669,555	491,833
Mobile Source	6,646,688	738,496	827,355	664,553	11,635,952	1,337,697	495,926
Total	17,132,419	1,318,227	1,520,041	1,050,448	55,226,197	4,396,897	1,638,518

Total HC = 63,832,101 Total NO_x = 18,450,646

Philadelphia Hydrocarbon Splits

Species	Carbon-Bond Fraction % as Carbon
PAR	74.0
OLE	2.8
ETH	4.1
ARO	13.2
CARB	5.9

This path is usually based on the wind fields in the first vertical layer only. As discussed earlier, the use of the wind fields in only the first layer can lead to differences in the maximum ozone predicted by the Systems Applications Trajectory model and the UAM on days with wind shear. For 13 July, the two highest observed ozone values occurred at both Conshohocken and Roxy Water Pump monitor. However, since the Roxy Water Pump monitor also had the highest predicted ozone value, it was used to determine the trajectory path to the ozone maximum for 13 July. The ozone value at Downington was used to determine the trajectory path to the ozone maximum for 19 July. Downington was chosen because in addition to having the highest predicted and a high observed ozone concentration, it was also estimated to be primarily influenced by the Philadelphia plume and not by the boundary conditions. The trajectory paths for the two modeling days are shown in Figures 10 and 11. Because the wind flow between the two lowest levels was important after 1100 EST on 13 July the average of the two levels was used to determine a trajectory path.

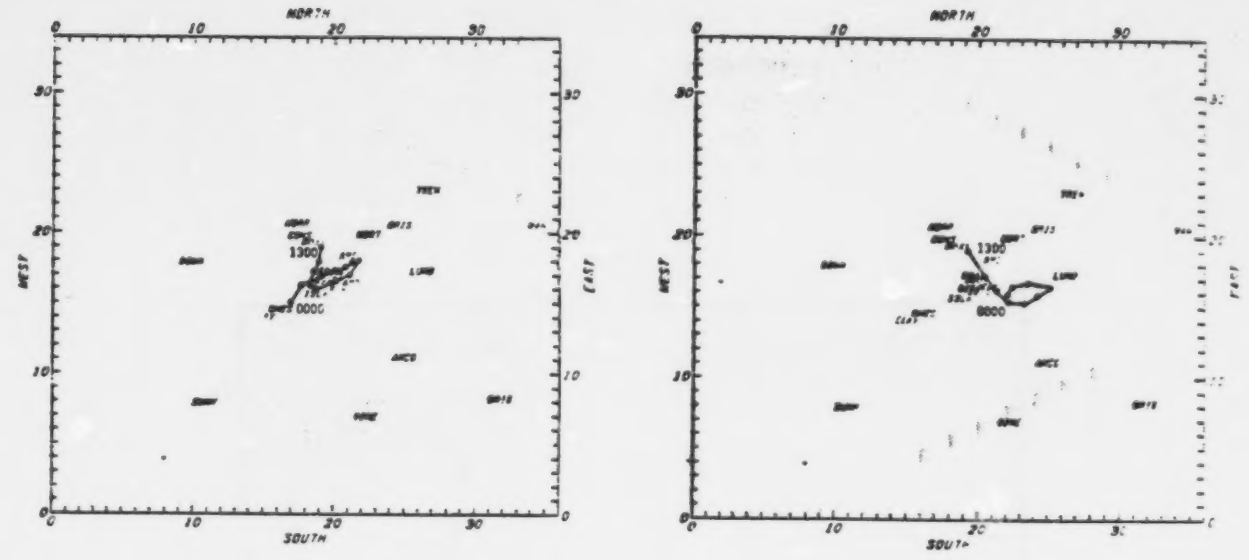
INPUTS USED IN THE LEVEL II OZIPM/CBM MODEL SIMULATIONS

Using the results of the Systems Applications Trajectory Model, emissions and meteorological conditions are constructed for a Level II type of EKMA model with Carbon-Bond chemistry (OZIPM/CBM). The Trajectory Model prints out the emissions and mixing heights along the trajectory path at hourly intervals. These mixing heights can be used as direct inputs to the OZIPM computer code. The emission rates from the Trajectory Model are in units of moles/hr for each of the Carbon-Bond species and are converted to ppmC/hr for volatile organic compounds (VOC) by the following equation:

$$\text{Emissions Rate (ppmC/hr)} = [24450/(Z_0 * 4000^2)][\text{Emissions Rate (moles/hr)}] \quad ,$$

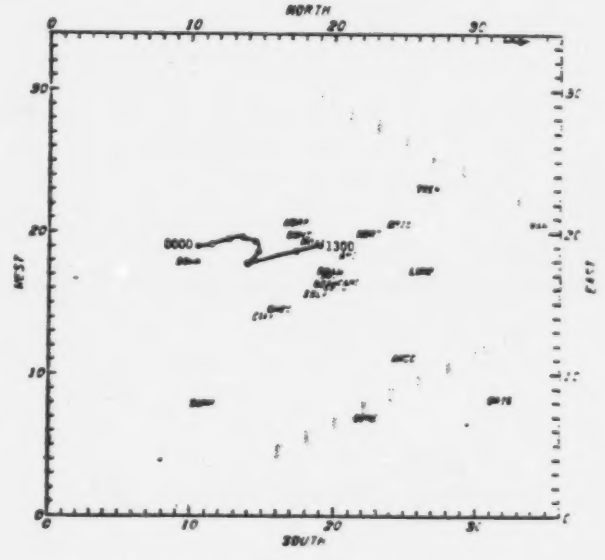
where Z_0 is the initial mixing height.

Initial NO_x and VOC precursors for OZIPM are determined from the initial conditions using the average of the layers below the mixing height in the Trajectory Model. NO_x and VOC precursors aloft are determined from the amount of precursors that entered the mixed layer from aloft in the Trajectory Model simulations. As a result, the OZIPM NO_x and VOC aloft precursors are often higher than measured values. The chemistry used in the Trajectory Model will produce secondary organic products (such as carbonyls) and ozone in the layer aloft. Thus, if we were to compare assumed aloft morning conditions in the CBM/OZIPM with actual morning measurements, concentrations may be higher for the OZIPM models. This



(a) Averaged trajectory

(b) Level I trajectory



(c) Level II trajectory

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FIGURE 10. Trajectory paths for 13 July 1979.

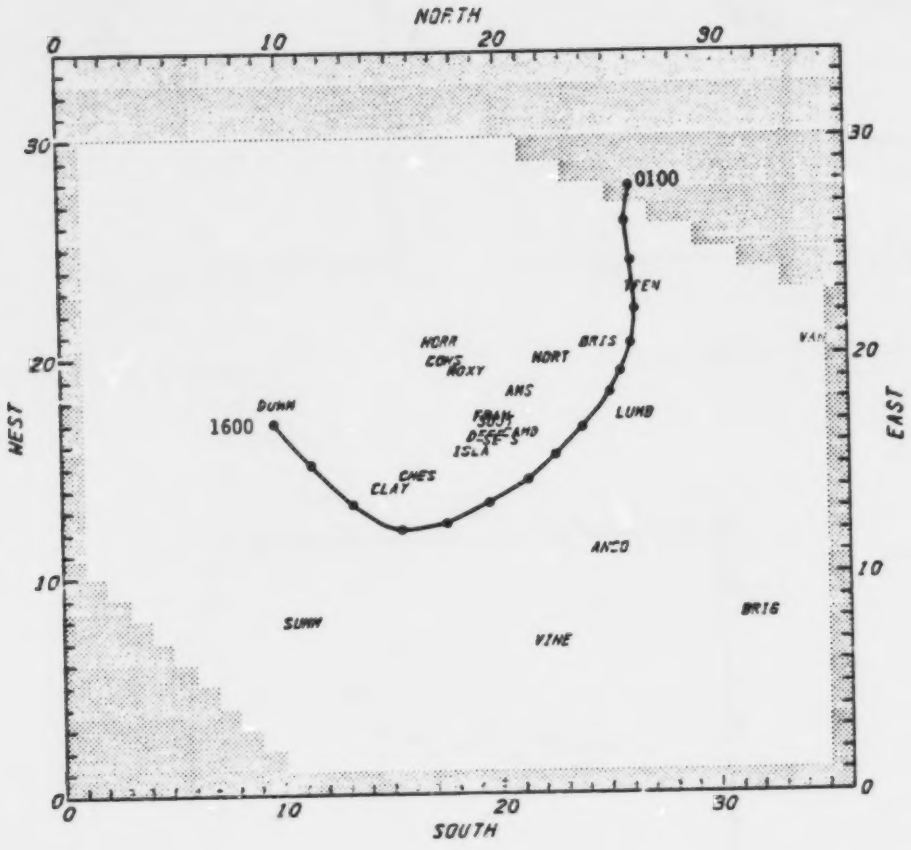

FIGURE 11. Trajectory path for 19 July 1979.

method was used because the species aloft continuously react in the Systems Applications Trajectory Model, whereas OZIPM does not treat precursors aloft until they are entrained in the late morning and early afternoon. Emissions and meteorological conditions for the two modeling days are shown in Tables 12 and 13.

INPUTS USED IN THE LEVEL III EKMA MODEL SIMULATIONS

Emissions and meteorological inputs were developed as outlined in the EPA (1981) guidelines document and used for the 1982 State Implementation Plan (SIP) for Philadelphia AQCR (DER, 1983). All assumptions made for this study are based on those documents. Six input options are available in the standard OZIPP Model (light intensity, dilution, ozone transport, precursor transport, post-0800 emissions, and reactivity). Emission inventories for the Philadelphia study developed by the EPA (1982) were reported for each county located in the study region. The county-wide emissions are presented in Table 14. The NO_x and VOC emissions in units of kg/day are converted to emission densities in units of kg/hr km^2. The initial conditions used in the level III EKMA calculations are presented in Tables 15 and 16.

TABLE 12. INITIAL CONDITIONS AND EMISSIONS RATES USED IN THE LEVEL II CBM/OZIPM CALCULATIONS FOR 13 JULY 1979

(a) Initial Conditions

Species	Surface	Aloft
NO_x	0.0253 ppm	0.0004 ppm
NMOC	0.7184 ppmC	0.0539 ppmC
O_3	0.0412 ppm	0.0775 ppm

NO_2/NO_x = .9922

Hydrocarbon reactivity: carbon fraction

	Surface	Aloft
OLE =	0.0277	0.0060
PAR =	0.7391	0.7148
ARO =	0.1311	0.0762
ETH =	0.0409	0.0311
CARB =	0.0612	0.1719

(b) Emissions Rates and Mixing Heights

Time (CDT)	Species VOC (ppmC/hr)	Species NO_x (ppm/hr)	Mixing Height at the Beginning of Each Hour (m)
0500-0600	0.0331	0.285	250.0
0600-0700	0.0802	0.359	250.0
0700-0800	0.4684	0.806	295.0
0800-0900	0.5557	0.1110	450.0
0900-1000	0.3221	0.0593	925.0
1000-1100	0.1800	0.0318	1200.0
1100-1200	0.1669	0.0255	1480.0
1200-1300	0.1528	0.0224	1480.0
1300-1400	0.1114	0.0248	1530.0
1400-1500	0.0802	0.0180	1530.0
1500			1420.0

TABLE 13. INITIAL CONDITIONS AND EMISSIONS RATES USED IN THE CBM/OZIPM CALCULATIONS FOR 19 JULY 1979

(a) Initial Conditions

Species	Surface	Aloft
NO_x	0.0073 ppm	0.0008 ppm
NMOC	0.1484 ppmC	0.0534 ppmC
O_3	0.0281 ppm	0.0611 ppm

NO_2/NO_x = 0.988

Hydrocarbon reactivity: carbon fraction

		Surface	Aloft
OLE	=	0.0267	0.0069
PAR	=	0.7358	0.7173
ARO	=	0.1275	0.0725
ETH	=	0.0404	0.0323
CARB	=	0.0697	0.1710

(b) Emissions Rates and Mixing Heights

Time (CDT)	Species		Mixing Height at the Beginning of Each Hour (m)
	VOC (ppmC/hr)	NO_x (ppm/hr)	
0500-0600	0.0284	0.1082	188
0600-0700	0.0384	0.0306	164
0700-0800	0.1349	0.0294	190
0800-0900	0.1559	0.0278	350
0900-1000	0.2214	0.0429	600
1000-1100	0.9076	0.0628	890
1100-1200	0.5303	0.0443	1094
1200-1300	0.0615	0.0087	1430
1300-1400	0.0394	0.0109	1437
1400			1332

TABLE 14. VOLATILE ORGANIC COMPOUND (VOC) AND NITROGEN OXIDES (NO_x) EMISSIONS BY COUNTY FOR 1980.

County	VOC (kg/day)	NO_x (kg/day)
Bucks	94,730	51,846
Chester	48,522	29,231
Delaware	115,193	77,268
Montgomery	81,967	47,094
Philadelphia	156,169	100,084
Burlington	41,400	55,700
Camden	54,900	54,100
Gloucester	87,900	52,600
Mercer	43,100	66,400
Salem	32,300	38,100
New Castle	103,400	140,523

TABLE 15. INITIAL CONDITIONS USED IN THE LEVEL III EKMA CALCULATIONS FOR 13 JULY 1979

(a) Initial Conditions

Species	Surface	Aloft
NO_x	0.0 ppm	0.0 ppm
NMOC	0.0 ppmC	0.0 ppmC
O_3	0.004 ppm	0.105 ppm

NO_2/NO_x = 0.25.

Hydrocarbon reactivity: standard OZIPP conditions.
Morning mixing height: 250 m at 0800 CDT.
Afternoon mixing height 1232 m at 1500 CDT.
$NMOC/NO_x$ at 0600 to 0900 CDT = 6.9.
Design $\hat{O}_3$ = 0.20 ppm at Roxborough (1400 CDT).

(b) Emissions Fractions

Time (CDT)	NMOC	NO_x
0800-0900	0.120	0.160
0900-1000	0.120	0.160
1000-1100	0.120	0.160
1100-1200	0.120	0.160
1200-1300	0.120	0.160

TABLE 16. INITIAL CONDITIONS USED IN THE LEVEL III EKMA CALCULATIONS FOR 19 JULY 1979

(a) Initial Conditions

Species	Surface	Aloft
NO_x	0.0 ppm	0.0 ppm
NMOC	0.0 ppmC	0.0 ppmC
O_3	0.03 ppm	0.032 ppm

NO_2/NO_x = 0.25.

Hydrocarbon reactivity: standard OZIPP conditions.
Morning mixing height: 250 m at 0800 CDT.
Afternoon mixing height: 1132 m at 1400 CDT.
NMOC/NO_x at 0600 to 0900 CDT = 6.9.
Design O_3 = 0.17 ppm at Roxborough (1400 CDT).

(b) Emissions Fractions

Time (CDT)	NMOC	NO_x
0800-0900	0.550	0.700
0900-1000	0.550	0.700
1000-1100	0.550	0.700
1100-1200	0.550	0.700
1200-1300	0.550	0.700
1300-1400	0.550	0.700

SECTION 3

COMPARISON OF MODEL RESULTS

This section presents a comparison of the absolute predictions for each of the models discussed in the previous sections. Results of the four models--UAM; Systems Applications Trajectory; Level II OZIPM (with CBM-II and CBM-III chemistry) and Level III EKMA (with CBM-II and Dodge chemistry)--are compared for 13 and 19 July 1979 in Tables 17 and 18. In these tables, HC stands for a hydrocarbon reduction; BKHC indicates a reduced background concentration from 0.0576 ppmC or higher to 0.033 ppmC hydrocarbons; and BKO_3 indicates a reduced background ozone from 0.06 ppm to 0.04 ppm, on 19 July and from 0.08 ppm to 0.04 ppm on 13 July.

A wind field with considerable shear between the two layers simulated within the mixed layer was used in the UAM simulations for 13 July day. An effect of such shear combined with the rapid mixing occurring during midday is to create considerable horizontal dispersion of emitted pollutants. Another effect is to create a pseudoslowing of the trajectory path determined from the vector average of the winds in these two lowest layers of the UAM. Figure 10a shows the vector-averaged path created from the paths defined by the winds in layers 1 and 2. Figures 10b and c show the paths to the same final point defined by using either layer 1 or 2, respectively. Since a thorough mixing occurs between these two layers on a time scale of only a few minutes, any emissions occurring in the vast area between the two paths shown in Figures 10b and c will influence the air simulated to arrive at the final common point at 1300 hours. Hence, the emissions along the path shown in Figure 10a are also considerably dispersed away from the common point shown.

The agreement between the UAM and Systems Applications' Trajectory Models based on emissions along the averaged path shown in Figure 10a is apparently fortuitous. Table 17 shows that the base case versions agree fairly well, but shows a consistent divergence between the models as the severity of controls is simulated.

A brief investigation into the effect of the precursor pathway of the 13 July day was conducted. The Trajectory Model simulates a moving column of air with a horizontal size identical to one grid square of the UAM.

TABLE 17. MODEL OZONE RESULTS (pphm) FOR PHILADELPHIA ON 13 JULY AT ROXY WATER PUMP MONITOR

Scenario	UAM	SAI TRAJECTORY	Level II EKMA		Level III EKMA*		Level III EKMA†	
			CBM-2	CBM-3	CBM-3	DODGE	CBM-3	DODGE
Observed	20.00							
Base Case	19.3	19.1	18.8	17.2	19.0	19.0	20.0	20.0
25% HC§	14.3		12.7	11.7	16.6	15.6	17.1	16.6
50% HC	11.5		7.7	7.3	14.5	12.0	15.1	12.0
75% HC	9.5	5.5	4.4	4.3	11.0	6.0	11.0	5.9
BKHC§	15.9		17.2	15.8				
25% HC•BKHC	11.3		11.1	10.3				
50% HC•BKHC	8.0		6.3	6.1				
75% HC•BKHC	6.0		3.6	3.5				
BKO3§	17.9		17.5	15.2				
25% HC•BKO_3	12.9		11.3	9.7				
50% HC•BKO_3	9.7		6.1	5.4				
75% HC•BKHC	7.4		2.9	2.6				
BKHC•O_3	14.5		15.9	13.7				
25% HC•BKHC•O_3	9.6		9.6	8.7				
50% HC•BKHC•O_3	5.8		4.8	4.2				
75% HC•BKHC•O_3	4.8		2.1	2.0				

* Ozone base case value is the UAM model predicted value.

† Ozone base case value is the observed value at the monitoring station.

§ HC = hydrocarbon reduction; BKHC = reduced background concentration from 0.0576 ppmC to 0.033 ppmC hydrocarbons; BKO_3 reduced background ozone from 0.08 ppm to 0.04 ppm.

TABLE 18. MODEL OZONE RESULTS (pphm) FOR PHILADELPHIA ON 19 JULY AT THE DOWNINGTON MONITOR

Scenario	UAM	SAI TRAJECTORY	Level II EKMA		Level III EKMA*		Level III EKMA†	
			CBM-2	CBM-3	CBM-3	DODGE	CBM-3	DODGE
Observed	15.70							
Base Case	14.1	14.9	14.9	15.6	14.2	14.2	15.7	15.7
25% HC	12.1		12.4	14.6	13.2	11.5	14.1	12.5
50% HC	10.0		9.9	13.1	11.0	7.3	10.7	7.5
75% HC	9.0		7.7	11.0	9.0	3.9	7.0	3.7
BKHC§	11.1		11.5	14.6				
BKO3§	13.4		14.0	14.4				
BKHC+O_3	10.3		10.5	13.0				

* Ozone base case value is the UAM model predicted value.
† Ozone base case value is the observed value at the monitoring station.
§ HC = hydrocarbon reduction; BKHC = reduced background concentration from 0.0576 ppmC to 0.033 ppmC hydrocarbons; BKO_3 reduced background ozone from 0.06 to 0.04.

Hence the only emissions that affect the Trajectory Model are those along the pathway within the horizontal area of one grid square. As Figures 10b and c imply, the wind shear in the 13 July UAM simulations mixes emissions from over a rather wide area.

Two simulations for 13 July were run using the Systems Applications Trajectory Model along pathways parallel to the one shown in Figure 10a but displaced one grid cell to either side. The center path result was 0.191 ppm ozone at 1300, as reported in Table 17; the two adjacent pathways produced similar and higher (near 0.25 ppm) results, respectively. Hence the choice of pathway resulted in fortuitous agreement with the UAM results. The choice of pathway can result in a fairly high diversity in emissions and the UAM predictions contained a large horizontal mixing component due to the wind shear.

In general, the UAM shows much less sensitivity to hydrocarbon controls than do the Systems Applications Trajectory Model and Level II OZIPM models used for the 13 July cases as presented in Table 19. The cause of the lower sensitivity may be related to the wind shear because the discrepancy shown for the 19 July cases (Table 20) is much less. Furthermore, there was good agreement in all other comparisons of trajectory models matched to UAM input (e.g., Whitten and Hogo, 1981; Killus and Whitten, 1983). The study of Killus and Whitten (1983) is especially noteworthy because the UAM was modified to use a significantly different chemical mechanism. Results of parallel control strategy simulations using the UAM and Level II OZIPM models agreed very closely when the chemistries were identical, even though the two chemical mechanisms predicted quite different responses to precursor controls. Hence, the wind shear in the 13 July simulation appears to influence the control strategy response. Unfortunately sufficient time and funding were not available for this study to confirm and elucidate the effect of wind shear on control predictions. Until this effect is studied more completely, the UAM results must be considered suspect since wind shear in the presence of rapid vertical mixing over long periods of time is difficult to justify physically and no data or physical evidence are available to support such wind shear on 13 July in the Philadelphia area.

Tables 19 and 20 show a difference in Level II OZIPM results for the CBM-II and CBM-III chemical mechanisms. Contract limitations did not allow investigation of these differences; however, it is noteworthy that on 19 July, the CBM-II mechanism is somewhat more sensitive to controls or background changes, whereas on 13 July, the two chemical mechanisms show similar sensitivity to hydrocarbon control.

Tables 17-20 also show predicted ozone and ozone reductions for the Level III (city-specific) EKMA using either the CBM-III or the standard

TABLE 19. PERCENT REDUCTION IN PREDICTED OZONE BETWEEN SCENARIOS AT ROXY WATER PUMP MONITOR FOR 13 JULY**

Scenario	UAM	SAI TRAJECTORY	Level II EKMA		Level III EKMA*		Level III EKMA†	
			CBM-2	CBM-3	CBM-3	DODGE	CBM-3	DODGE
Base Case	-	-	-		-	-	-	-
25% HC§	26		32	32	13	18	15	17
50% HC	40		59	58	24	37	25	40
75% HC	51	71	77	75	42	68	45	71
BKHC§	18	-	9	8	-	-	-	-
25% HC•BKHC	41	-	41	40	-	-	-	-
50% HC•BKHC	59	-	66	65	-	-	-	-
75% HC•BKHC	69	-	81	80	-	-	-	-
BKO_3§	7	-	7	12	-	-	-	-
25% HC•BKO_3	33	-	40	44	-	-	-	-
50% HC•BKO_3	50	-	68	69	-	-	-	-
75% HC•BKO_3	62	-	85	85	-	-	-	-
BKHC•O_3	25	-	15	20	-	-	-	-
25%•BKHC	50	-	49	44	-	-	-	-
50%•BKHC	70	-	74	76	-	-	-	-
75%•BKHC	75	-	89	88	-	-	-	-

* Ozone base case value is the UAM model predicted value.

† Ozone base case value is the observed value at the monitoring station.

§ HC = hydrocarbon reduction; BKHC = reduced background concentration from 0.0576 ppmC to 0.033 ppmC hydrocarbons; BKO_3 reduced background ozone from 0.08 ppm to 0.04 ppm.

** All percent reductions are expressed relative to base case ozone level.

TABLE 20. PERCENT REDUCTION IN PREDICTED OZONE BETWEEN SCENARIOS AT DOWNINGTON MONITOR FOR 19 JULY**

Scenario	UAM	SAI TRAJECTORY	Level II EKMA		Level III EKMA*		Level III EKMA†	
			CBM-2	CBM-3	CBM-3	DODGE	CBM-3	DODGE
Base Case	-	-	-	-	-	-	-	-
25% HC§	14	-	17	6	7	19	10	20
50% HC	29	-	34	17	23	49	32	52
75% HC	36	-	48	29	37	73	55	76

* Ozone base case value is the UAM model predicted value.
† Ozone base case value is the observed value at the monitoring station.
§ HC = hydrocarbon reduction.
** All percent reductions are expressed relative to base case ozone level.

Dodge chemistry. Two sets of results are presented in Tables 17 through 20 for each city-specific EKMA model (with CBM-III or Dodge chemistry). The first set compares city-specific EKMA predictions based on ozone design value (base case) similar to the UAM-predicted ozone. This set allows comparison of the city-specific EKMA with more sophisticated models even though the inputs differ. The second set of city-specific EKMA results is based on the observed ozone at the monitoring station. This set of results would have been obtained under regulatory analysis of the two modeled days and provides a comparison of the UAM and city-specific EKMA as regulatory tools. In these comparisons, the Level II OZIPM can also be called city-specific EKMA in the sense that alternate procedures, as outlined in the city-specific EKMA guidelines (EPA, 1981), are applied for the two modeled days.

Tables 18 and 19 present absolute ozone predictions for the city-specific EKMA compared to those of more sophisticated models for 13 July and 19 July 1979. For the city-specific EKMA simulations using CBM-III, the nominal default precursor background was assumed as transport conditions (EPA, 1984). Since city-specific guidelines were applied for these comparisons, no attempt was made to simulate the scenarios in which background conditions were altered along with the emission changes.

Tables 19 and 20 show the percent reduction in ozone predicted by the city-specific EKMA models. From Tables 19 and 20 we see that the city-specific EKMA is less sensitive to hydrocarbon reductions for both modeled days compared to the UAM and trajectory models when the CBM-III is used. When the Dodge chemistry is used in the city-specific EKMA, a greater sensitivity to hydrocarbon controls is shown for both modeled days.

Estimates of the VOC reductions needed to lower peak ozone to the level of the National Ambient Air Quality Standard (NAAQS) of 12 pphm are shown in Table 21. For the July 13 day (considering no change in boundary conditions), the UAM VOC estimate is 45 percent. The control estimates of the Level II models are lower than those of the UAM (when there are no changes in the boundary conditions) for both carbon-bond mechanisms. We see from Table 21 that both CBM-2 and CBM-3 give similar control estimates for the different sensitivity scenarios. The Level II models (CBM-2 and CBM-3) predict lower control estimates for the case in which background O_3 is reduced concurrent with emission reductions. For cases in which background HC is reduced concurrent with emission reductions and when both HC and O_3 are reduced concurrent with emission reductions, the Level II models predict control estimates similar to those of the UAM. With the Level III approach, the control estimates obtained with the Dodge mechanism are slightly higher than those of the UAM (50 percent versus 45 percent), while the CBM-3 estimates are higher yet (70 percent and 69 percent versus 45 percent). Note also that there is little difference

between results obtained using the predicted UAM base case peak ozone or the observed peak in the Level III analyses on this day because they are very similar in value (19.3 pphm versus 20.0 pphm, as shown in Table 17).

The results are more mixed for July 19, 1979, however. The UAM estimate is 25 percent. The Level II estimates differ significantly, depending upon the mechanism that is used (24 percent and 42 percent for the CBM-2 and CBM-3, respectively). Further investigations of the Level II simulations for 19 July show that the chemistry of excited singlet state oxygen atoms ($O^{'D}$) formed from ozone photolysis (which is accounted for in CBM-3, but not in CBM-2) can lead to very different control estimates. The $O^{'D}$ chemistry can have a major effect when NO_x concentrations are high during the late afternoon hours of the simulation, as in the case of the 19 July simulations. For the Level III analyses, the control estimate obtained with the Dodge mechanism is slightly lower than the UAM estimate when the same base ozone value is used (19 percent versus 25 percent), but slightly higher when the observed ozone value is used as the base. The CBM-3 mechanism, when used in the Level III analysis, produces control estimates that are higher than either the UAM estimates or the Level III/Dodge estimates, regardless of the base case ozone.

A comparison of the model estimates presented in Table 21 provides some insight into the results that might be obtained if the results were used in a regulatory analysis. Several caveats are in order however. First, since only two days were analyzed, it is very difficult to discern any general patterns. The inclusion of more days is precluded by the lack of UAM simulations. Second, the VOC reductions shown in Table 21 correspond to peaks measured at single monitoring sites (i.e., the Roxy Water Pump for 13 July and Downington for 19 July). The UAM estimates of VOC reduction needed to lower peak ozone in the entire region to 12 pphm are higher (Braverman and Haney, 1985). Also, the limited number of days analyzed with the UAM make it difficult to assess definitively the differences that might actually occur in a true regulatory analysis. For example, the State Implementation Plan (SIP) for ozone (DER, 1983) estimated that 44 percent reduction in VOC would be required to achieve the standard. This estimate was obtained from a detailed city-specific EKMA analysis (using Dodge chemistry) of ozone data collected at 10 air quality monitoring stations over the three-year period of 1979-1981. The design ozone was 0.171 ppm at Trenton, New Jersey, on 24 June 1980. Therefore, the 13 July and 19 July 1979 days evaluated in this study might not correspond to the final design used in regulatory planning.

TABLE 21. HYDROCARBON EMISSION REDUCTIONS REQUIRED TO MEET THE NAAQS FOR OZONE FROM THE SENSITIVITY SIMULATIONS OF 13 AND 19 JULY

	13 July Attainment Level							19 July Attainment Level						
	Level II†			Level III†		Level III**		Level II†			Level III†		Level III**	
Sensitivity Simulation	UAM	OZIPM/ CB-2	OZIPM/ CB-3	CB-3	DODGE	CB-3	DODGE	UAM	OZIPM/ CB-2*	OZIPM/ CB-3*	CB-3	DODGE	CB-3	DODGE
No change in boundary conditions	45	32	32	70	50	69	50	25	24	42	40	19	43	31
Reduction in O_3 background concurrent with emission reductions	38	24	24	-	-	-	-	-	-	-	-	-	-	-
Reduction in HC background concurrent with emission reductions	23	23	27	-	-	-	-	-	-	-	-	-	-	-
Reduction in both O_3 and HC background concurrent with emission reductions	19	18	19	-	-	-	-	-	-	-	-	-	-	-

* Reduction scenarios for EKMA were not run because the background reductions in the airshed scenarios were done on the horizontal east and northeast boundaries, and EKMA is unable to model the horizontal boundaries.

** Base case ozone value based on observed value at monitoring station.

† Base ozone value based on UAM predicted base case ozone.

SECTION 4

SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

SUMMARY

EKMA was evaluated primarily by comparing the box model (OZIPM) that forms its basis with more sophisticated models in applications to the Philadelphia area. The study was carried out at several levels, beginning with evaluation of OZIPM and ending with an evaluation of the control-strategy predictions resulting from application of the city-specific EKMA (OZIPM) based on EPA guidelines (EPA 1984). The OZIPM model was compared with the UAM and Systems Applications Trajectory model, as well as with modified versions of the original OZIPM model. The basic OZIPM model is a simple moving-air-parcel, or box, model that can be used with any chemical mechanism. The OZIPM model treats time-dependent, precursor-emission factors and expansion of the air parcel; entrainment is treated by assuming constant concentrations outside the parcel.

CONCLUSIONS

The primary emphasis of this comparison study was the identification of features in the basic OZIPM model that could explain differences between the results of the OZIPM model and those of other models. For the most part, the study used UAM data files to generate appropriate OZIPM inputs. The use of these files allows the comparison of models having a common data base and comparison of EKMA simulations for regulatory analysis: OZIPM can be run using either UAM inputs or by following EPA guidelines (EPA, 1981, 1984).

This study and similar studies by Whitten and Hogo (1981), Whitten et al. (1981) and Hogo et al. (1981) using data for Los Angeles, San Francisco, Sacramento, and Tulsa show that the OZIPM model can provide results that are often quite similar to those of the more complex models. By identifying specific differences in model formulation and analyzing intermediate results, the formulation feature that produced the difference in the results of two models could often be isolated. Even though the absolute values predicted by the OZIPM model can differ significantly from those of the more complex models (such differences can result from the

different chemical mechanisms employed), EKMA isopleths (which use OZIPM results) typically yield control predictions that correspond with those of the more complex models.

The main conclusions reached in the comparison of UAM and OZIPM results in application to the Philadelphia area are similar to those of previous studies (e.g., Whitten et al., 1981):

(1) These two models tend to show close agreement.

(2) Any box model (e.g., OZIPM) when run in conjunction with a grid model (e.g., UAM), can serve as a useful and inexpensive tool for understanding, analyzing, and evaluating important and sensitive elements of the situation being modeled.

(3) The Systems Applications Trajectory Model serves as a source of data for the EKMA type models, as well as an important conceptual link between these models and the UAM.

Comparisons of the Systems Applications Trajectory Model and an EKMA-type model (OZIPM/CBM) modified to most closely resemble the Systems Applications Trajectory Model showed that many features in the Systems Applications Trajectory Model can often be eliminated or simplified with a minimal effect on results. For instance, the two levels within the mixed layer of the Systems Applications trajectory model seem adequately represented by a single layer in the OZIPM/CBM model. The same photochemical kinetic mechanism, the Carbon-Bond II Mechanism (Whitten et al., 1980), is used in the UAM, the Systems Applications Trajectory Model, and the OZIPM/CBM model. For comparison, the OZIPM/CBM was also run with CBM-III chemistry (Killus and Whitten, 1984).

For the 1982 SIP studies, the EPA categorized degrees of model sophistication by Levels I through IV (pages 65669-65670 of the 14 November 1979 Federal Register). The Level I models used in this study are the UAM and the Systems Applications Trajectory Model. Versions of the OZIPM box model used in this study that use trajectory paths based on UAM inputs are considered to be Level II EKMA models. Level I and Level II models are distinguished by the degree of complexity. Briefly, Level I models use gridded data, whereas Level II models use data from only those grids that the trajectory path passes through. A trajectory model can be classified as either a Level I or Level II model based on its level of complexity. The primary feature that defines a Level III EKMA model is the assumed trajectory relating early-morning urban precursors to an observed ozone peak (EPA, 1981).

Level III EKMA simulations that showed reasonable agreement with observations were also performed. However, the use of county-wide emissions in this model makes detailed comparisons with the other models used in this study difficult because their emissions data differ.

RECOMMENDATIONS

The following considerations are suggested for future studies:

For cases in which differences in the control strategy predictions of various models are found to be related to differences in their chemistry, it is important to investigate the chemical reactions that produce these differences. Where appropriate smog chamber experiments that would validate one or more types of chemical mechanisms can be identified, these experiments should be performed.

The use of more complex models such as the UAM should be accompanied by the use of EKMA, both for absolute trajectory simulations along the path to the major ozone peaks, and to obtain control strategy guidance from the EKMA isopleth diagrams. The studies performed to date show that unless the wind fields are complicated by such factors as wind shear, the two types of models normally give similar results. In the absence of complex meteorological factors, important differences in results would indicate the existence of problems in one or both of the models that should be investigated.

Identification of background concentrations and reactivities must be carefully considered for both present and future simulations. Severe control requirements can be implied if the level of background pollutants is overstated.

The regular city-specific algorithm might be modified to allow optional starting times in place of the present 0800 LDT starting time. Earlier starting times would emphasize dependence on an emissions inventory, whereas later starting times might emphasize dependence on initial conditions.

Modifications to the current version of the EKMA have also been suggested in other studies. Although such suggestions have not been addressed in this study, their implementation might also be considered:

(1) Isopleths based on emissions inventories might be further developed to perhaps replace the present initial-condition-based isopleths (Hogo, et al., 1981). Urban HC and NO_x

measurements are often not relevant to the initial trajectory. Trajectories might originate prior to the present 0800 LDT time. Mathematically, path definition is not important to moving-air-parcel models unless differences in emission density and mixing height exist. Preliminary calculations suggest that precise definition of mixing height prior to 0800 is unimportant. Wind velocities prior to 0800 are typically low, so that few grid squares would be crossed before the arrival of the air parcel at the more easily definable trajectory paths now used, i.e., those beginning at 0800 hours. Therefore, an important factor in the success of an emissions-dominated model would be minimal (or at least moderate) diversity of the emissions density in the vicinity of the present 0800 starting area. In the present study, the path defined by the average of the winds in the first two layers passed over significant emissions sources, but the paths defined by winds in the surface and second layers were on either side of the main emissions sources. Since models are often for episodic conditions, the path must be forced over major emissions if the early morning winds are uncertain and significant emissions diversity exists.

An emissions-oriented model may also be potentially more advantageous than the present initial-condition-and-measured-HC/NO_x model because of the poor mixing that can occur prior to 0800. Measured urban HC and NO_x values often vary widely, even when taken at the same location, as a result of local mixing and local emissions. Use of the HC/NO_x ratio does not necessarily mitigate the problem because the measured ratios can still be dominated by local emissions and mixing effects. Starting the model earlier and filling it with well-mixed emissions from the region upwind of, and within, the main urban area may provide a more realistic simulation of the air that arrives at the downwind site where the ozone maximum occurs. Furthermore, the ordinate and abscissa (which are scaled relative to the emissions rather than to the initial concentrations) would relate more closely to the purpose of the EKMA (i.e., to estimate the changes in peak ozone concentrations resulting from changes in emissions).

The use of any atmospheric model under conditions of wind shear within the mixed layer should be approached with caution and extensive confirmation. Although Level II box models are basically inappropriate under such conditions, their use to assess a specific area can

still be helpful in Level I grid model studies. For example, by using averaged wind data, a box model can be used to determine a preliminary trajectory. The results from this trajectory can be used to assess input data to the airshed.

A generalized concept can be associated with EKMA that goes beyond its present specific formulation and uses; developmental work should be continued to update its formulation and improve and broaden its utility. Specifically, the following steps are suggested:

(1) Point source emissions might be handled so that their interaction with all possible urban HC/NO_x concentrations could be evaluated as part of a new-source review procedure.

(2) Percent cutback diagrams (PCD) might be added to the OZIPM code so that both the isopleth and the PCD are generated. A PCD is a diagram of ozone isolines, but the ordinate and abscissa represent the percent control of NO_x or VOC required to meet the 0.12 ppm O_3 standard using the EKMA procedure. A VOC/NO_x ratio is required to generate a PCD. Such a diagram graphically illustrates all possible combinations of VOC and NO_x control implied by the EKMA procedure to reach the 0.12 ppm O_3 line on a regular EKMA ozone isopleth diagram.

(3) Statistical packages could be combined with EKMA to generate the probable number of exceedances resulting from various control scenarios.

(4) Isopleths of many species other than ozone could be useful. Some candidates are nitric acid, hydrogen peroxide, and sulfate species relevant to acid deposition. Also, toxic species (e.g., formaldehyde) can be studied using the generic-model-and-isopleth approach.

(5) A "two-stage" version of EKMA should be further developed. Local authorities can effectively control only stationary sources, whereas mobile sources tend to be controlled at the federal level. Hence, a first-stage EKMA would vary only mobile emissions and the second stage would vary only stationary emissions. This would give local authorities a much clearer picture (isopleth) of the effectiveness of stationary source controls. Also, the difference in reactivity between mobile and stationary sources could be more accurately modeled using the staged EKMA.

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APPENDIX

DESCRIPTION OF INPUTS USED IN URBAN AIRSHED MODEL SIMULATIONS

The following description of the inputs used in the Urban Airshed Model (UAM) simulations are taken from Braverman and Haney (1985). As discussed in the main volume of this report, many of the inputs derived for less complicated models are based on the inputs developed for the UAM.

MODELING REGION SPECIFICATIONS

The modeling region of the Philadelphia airshed specified in this study is 180 x 170 km, or a total area of 30,600 km^2. This region covers parts of Pennsylvania, Delaware, Maryland, and New Jersey and includes the metropolitan areas of Philadelphia, Pennsylvania; Wilmington, Delaware; and Trenton, New Jersey (see Figures 1 and 2).

The modeling region specifications (e.g., grid origin, grid size, number of horizontal cells, etc.) are contained in what is known as the REGION packet. For the Philadelphia application, the modeling grid contains 36 by 34 horizontal cells that are fixed at 5000 m by 5000 m, and 4 vertical cells (layers) that vary in thickness depending on the hourly mixing height and the height of the top of the modeling region. There are two vertical cells below and above the mixing height. During the simulations, the cells, or layers, below the mixing height may attain the minimum cell thickness specified (for this application, 50 m) during the night when the mixing height is at a minimum. As the mixed layer thickens during the day, the vertical thickness of layers 1 and 2 grows, while the thickness of the upper layers (3 and 4) decreases. The specified height for the top of the modeling region is fixed for each hour and is used in preparing the REGIONTOP file. The UAM REGION packet in all input files was specified as follows:

```
UTM ZONE:   18
X ORIGIN: 387000 m EASTING
Y ORIGIN:   4340000 m NORTHING
GRID SIZE:  5000.0 m
```

TOP OF REGION: 1630.0 m
NX: 36 cells
NY: 34 cells
NZ: 4 cells
MINIMUM CELL THICKNESS-LOWER LAYERS: 50 m
MINIMUM CELL THICKNESS-UPPER LAYERS: 50 m

PREPARATION OF INITIAL AND BOUNDARY CONCENTRATION INPUTS

Three input files--AIRQUALITY, BOUNDARY, and TOPCONC--are required for the specification of initial and boundary conditions of all pollutants. The AIRQUALITY file specifies the concentrations of all species for all grid squares at the start time of the run. The data available for this file is constructed using monitoring data from 16 surface air quality sites, 18 surface meteorological sites, and 3 upper-air meteorological sites. In addition, for this application a helicopter was employed to collect air quality and meteorological data above the surface in an attempt to quantify pollutant transport aloft. Within the Philadelphia urban area, special stations were also established for the collection of hydrocarbon data. Two methodologies were used for constructing gridded fields of initial conditions from these data--one for constructing the gridded ground-level concentrations and one for extrapolating the concentrations aloft from the ground-level values.

To construct the initial and boundary concentration files, the Philadelphia air quality data base were examined to characterize the levels and distribution of pollutants in the study area. This information was used to identify pollutant concentrations and to establish methodologies for preparing these inputs. The available NO_x and ozone data collected at the 16 surface air quality stations were generally adequate to characterize the ground-level initial and boundary values for these pollutants. Inputs to the simulation (e.g., wind fields, mixing heights) were prepared after examining day-specific air quality and meteorological data collected from the network of stations in the region. To simulate the carryover of emission precursors on 13 July from the previous day, ozone readings at the Vineland, New Jersey monitor along the southeast boundary of the simulation grid were used to specify hourly ozone boundary conditions.

An early-morning (0000-0700 EST) nonmethane hydrocarbon (NMHC) concentration of 0.15 ppmC was specified for cells below the mixing height, based on an analysis of data from other Northeast Urban Corridor cities under similar meteorological conditions (stagnation and carryover). The hydrocarbon species split of NMHC was chosen to represent an aged urban air mass as recommended by Killus (1982). This value, along with those

for NO, NO_2, and PAN (specified after examining late-afternoon downwind observed data at Downington, Pennsylvania and Van Hiseville, New Jersey for days on which these sites were influenced by the Philadelphia urban plume), were used as input to the EKMA/OZIPM trajectory model to obtain the daytime variation of these species for use as hourly boundary conditions along the southeast inflow boundary. The OZIPM simulation predicted ozone values similar to those recorded at the Vineland monitor, thus giving credance to these boundary condition values.

On 19 July, observed NO and NO_2 data for the hour of 0500-0600 EST were used as input values for the northeast and east boundaries below the mixing height for the hours of 0000-0600 (Braverman and Haney, 1985). Since hydrocarbons were not measured at the Van Hiseville monitor, estimates of the influx of total reactive hydrocarbons across the northeast and east boundaries below the mixing height were specified by multiplying the hourly NO_x concentrations at the Van Hiseville monitor by the Philadelphia surface layer emission inventory hydrocarbon/NO_x ratio of 6. The total reactive hydrocarbon value was then speciated into Carbon-Bond Mechanism components, using the carbon-bond fractions of the emission inventory.

Preparation of Gridded Ground-Level and Aloft Initial Concentration Fields

Initial conditions for all species were specified using all available monitoring data in the Philadelphia region. The simulation of 13 July commenced at midnight, requiring concentration values corresponding to this time. Rather than using the hourly averaged observed value for each species for the midnight hour, initial condition concentrations were calculated for each monitor by averaging the observed hourly average pollutant concentrations from 2300-2400 EST on 12 July with the 0000-0100 EST concentration on 13 July to obtain a two-hour averge value for midnight. A Poisson interpolation routine was used to construct the gridded surface fields.

Sixteen surface air quality stations were used to estimate NO, NO_2, and O_3 ground-level concentrations. In past modeling applications it was sometimes necessary to add stations in the corners of the modeling region and to give these stations background values that reflect the rural nature of the outlying portions of the grid. However, in this study, initial conditions for surface grid cells without monitors were obtained by employing a Poisson interpolation, which extrapolates these values using data collected in the more source-intensive portions of the grid. After the surface field was computed, a vertical interpolation method was chosen in which the background concentration at the top of the modeling region

(TOPCONC) was used in levels 3 and 4, and the level 2 value was obtained by a linear interpolation between the surface value and the level 3 value. Using this method, all grid cells in all levels were initialized with appropriate concentrations for all species.

The amount of spatial variation in the early-morning NO_x and O_3 monitoring data differed from day to day. For 13 July, the NO_x data ranged from 0.003 ppm at Summit Bridge to 0.127 ppm at the downtown Camden site. The Camden observations exhibited the highest early-morning NO_x concentrations. The NO_x measurements for 19 July were lower, with a range of 0.006 to 0.080 ppm.

PREPARATION OF METEOROLOGICAL INPUTS

The meteorological inputs to the UAM determine the transport characteristics and rate of mixing of the pollutant cloud. Meteorological factors often account for violation of the NAAQS on some days and not on others, even when the emissions patterns are similar. Therefore, the wind field and the hourly mixing depths are important UAM inputs. Since upper air meteorological data were collected in Philadelphia only on a limited number of special study days, the three-dimensional structure of the wind field was one of the most difficult inputs to specify.

Calculation of The Wind Field

Similar to the construction of the initial conditions, the three-dimensional wind field was calculated in two steps: The surface wind field was prepared first, followed by the upper-level wind fields. The surface wind field was developed using the ground-level measurements and synthesized data, and an interpolation routine that weights the observations by the inverse of the distance from the grid square. Mathematically, this relationship can be written:

$$\bar{u}_k = \frac{\sum_{i=1}^{n} u_i r_{ik}^{-1}}{\sum_{i=1}^{n} r_{ik}^{-1}} ,$$

$$\bar{v}_k = \frac{\sum_{i=1}^{n} v_i r_{ik}^{-1}}{\sum_{i=1}^{n} r_{ik}^{-1}} \quad ,$$

where $\bar{u}_k$ and $\bar{v}_k$ are the calculated horizontal velocity components for grid cell k; u_i and v_i are the measured velocity components at station i; n is the number of wind measurements; and r_{ik} is the distance between monitoring site i and grid cell k. A smoothing algorithm, which replaces each of these velocity components by the average velocity component calculated over the block of nine surrounding cells, was used to smooth the calculated wind field to eliminate any discontinuities introduced by the interpolation procedure. Finally, the average measured wind speed and the average computed wind speed was calculated over the modeling region resulting from the preceding calculations. The wind speed in each grid cell was then scaled by the ratio of the average measured speed to the average computed speed because the vector-averaging processes embedded in the interpolation and smoothing steps yield wind speeds lower than the observations.

Observed surface wind data were available at the following locations:

Station	UTM Easting (km)	UTM Northing (km)
Northeast Philadelphia Airport, Pennsylvania	499.0	4436.0
Philadelphia International Airport, Pennsylvania	478.6	4414.6
McQuire Air Force Base, New Jersey	534.1	4431.3
Willow Grove Naval Air Station, Pennsylvania	488.7	4449.8
Lakehurst Naval Air Station, New Jersey	556.9	4431.5
Trenton-Mercer County Airport, New Jersey	515.6	4459.0
Millville Airport, New Jersey	494,3	4357.0
Greater Wilmington Airport, Delaware	448.6	4390.7
Chester, Pennsylvania	467.8	4409.3
Bristol, Pennsylvania	510.0	4439.5
Allegheny-Philadelphia, Pennsylvania	491.7	4425.2
Summit Bridge, Delaware	441.0	4376.0
Downington, Pennsylvania	436.0	4426.0
Lumberton, New Jersey	518.0	4423.0
Van Hiseville, New Jersey	559.0	4439.5
Norristown, Pennsylvania	473.5	4440.0
NW	430.0	4480.0
NE	550.0	4490.0
SE	535.0	4380.0
SW	410.0	4360.0

The last four stations in this list were the designated "pseudo stations" used to fill the gaps in the observed surface field before the interpolation procedure was used.

The next step in the wind field preparation involved an interpolation program to obtain a complete surface wind field. The program WINTER employed a $1/R^2$ interpolation scheme and used the screened observation file to create a gridded surface wind field. Preparation of the winds in the upper layers was the next step in the process.

Although they were performed on other days during the 1979 Philadelphia Oxidant Study, upper-level atmospheric measurements were not performed on 13 July in central Philadelphia. Consequenty, the nearest upper-level radiosonde data for this day correspond to the twice-daily releases at JFK and Dulles airports. These data were carefully analyzed to establish their utility for prescribing upper-level wind and temperature fields over Philadelphia, and confirm the existence of a southwesterly through northwesterly synoptic flow, which is apparent from an examination of the NWS daily weather map for this day (see Figure 3). On the basis of these four soundings, the 1900 EST sounding of 12 July, and the 0700 EST sounding of 14 July, an attempt was made to estimate average synoptic-level (i.e., ≅ 1500 m) wind velocities at JFK and Dulles for the entire day. This was achieved by averaging the radiosonde values over a range of 1200 to 1800 m for each sounding. Hourly estimates of winds aloft were derived using vector interpolation between soundings. This review of both sets of soundings resulting in the selection of a constant vector to be used for each hour to describe the level-4 winds.

To obtain wind vectors for levels 2 and 3 for 13 July, the program WINDCHANG was used. This program performed a linear vector interpolation to obtain the vectors for levels 2 and 3 using the surface vector and the level 4 vector for each grid cell. The program read the REGIONTOP and DIFFBREAK mixing height files to determine the height of the node for each level for each hour. These files were read because the mixing height changes hourly and determines the thickness of each vertical cell. After the node heights were determined for levels 2 and 3, a linear interpolation was performed to compute the mid-level direction. The speed of the level 2 or level 3 vector was then increased by employing a power law equation as follows:

$$V_2 = (V_4 - V_1)*(NODE_2/1500)^{\alpha} + V_1$$

$$V_3 = (V_4 - V_1)*(NODE_3/1500)^{\alpha} + V_1$$

where

$NODE_2$ = the height of the node of level 2,

$NODE_3$ = the height of the node of level 3,

V_4 = the speed of the vector for level 4,

V_1 = the speed of the vector of the surface wind, and

$\alpha = 0.2$

This method is only one means of interpolating for the winds in levels 2 and 3. In this equation, α is the surface friction coefficient that varies as underlying features on the surface vary. If the α coefficient had been dropped, a straightforward linear interpolation would have resulted from the equation; however, the magnitude of the winds in levels 2 and 3 would have been underestimated with this procedure. Only one value of α was used in this application to reflect an average value of surface friction throughout the region. A nonlinear interpolation could also have been used by solving for α in each grid cell and using the resulting α in the interpolation; however, this method was not used in this application.

A full three-dimensional flow field was thus created for each hour. Either because of noise in the wind sampling network, or because of the nature of the vectors sampled at two distinct points, the resulting flow field contains a great deal of divergence. If the field is employed by the Urban Airshed Model with the divergence left in, spurious artificial vertical motions will result in unrealistic vertical transport. The last phase of the wind field preparation involves the elimination of nearly all divergence.

The program DIVFREE was written to read the three-dimensional file and eliminate most of the divergence in the flow field. This program was adopted from an EPA algorithm developed by Clark and Eskridge (1977) and is the final step in the creation of the wind field. As a quality control check, the wind vectors are then plotted on the airshed grid and examined for reasonableness before use in the Urban Airshed Model simulation. Trajectory analysis can be performed using this final file to determine the origin both in space and time of the parcels affecting the peak ozone concentrations.

Because of the availability of upper-air data within the airshed region on 19 July, the procedure used for specifying winds in levels 2, 3, and 4 differed from that used for the upper-level winds for 13 July.

Radiosonde or pibal wind measurements were available for three sites: Wilmington, Delaware, Downtown Philadelphia, and Trenton, New Jersey. These data were plotted graphically for review purposes. Figures A-1, A-2, and A-3 present measured winds aloft up to 3250 m above Wilmington, Downtown Philadelphia, and Trenton, respectively for 1200 EST on 19 July. The data plotted in these figures show a light surface flow (2 to 4 m/s) in a general southeasterly direction, while the wind speeds aloft (1250 to 3000 m) were moderate with a general westerly direction. All available upper-level wind data were plotted in this manner and utilized to estimate specific hourly inputs for each level. After examining the data, a constant average wind vector was obtained for each hour for levels 2, 3, and 4.

Mixing heights for 13 July 1979 were estimated every half hour for urban and rural areas for daytime, transitional, and nighttime regimes. Urban and rural mixing height cell designations are included in the discussion of the terrain file, page A15. Since no soundings were available for Philadelphia on this day, the daytime mixing heights between 0600 and 1400 EST were estimated using the available morning (0700 EST) and evening (1900 EST) radiosonde soundings at JFK and Dulles airports. The procedure used to estimate daytime mixing heights is similar to the methodology used by Holzworth (1972). First, spatially averaged surface temperatures for the Philadelphia region were computed for each hour using all available meteorological measurement sites. The resultant average hourly surface temperatures were plotted on temperature-versus-height graphs of each sounding. The height of the intersection between the dry adiabat of the surface temperature and the temperature sounding was then taken as an estimate of the mixing height.

Between 0600 and 1200 EST, the mixing height was computed as the average of the values estimated from the JFK and Dulles airport morning soundings. An average of the JFK and Dullas morning and afternoon soundings was used to compute mixing heights between 1200 and 1400 EST. An exception to this procedure was made for estimating rural mixing heights between 0600 and 0900 EST, before the dissipation of the rural surface stable layer. During this period rural mixing heights were subjectively estimated to increase from the overnight value of 100 m to the 0900 EST value. Because of the general nature of the "adiabatic" procedure used for estimating daytime mixing heights, no other distinction was made between urban and rural mixing heights during the 0600-1400 EST time period.

The overnight (0000 through 0600 EST) mechanically dominated mixing heights were set to a constant value of 250 m in urban areas and 100 m in rural areas. These "default" values were obtained from analyses of

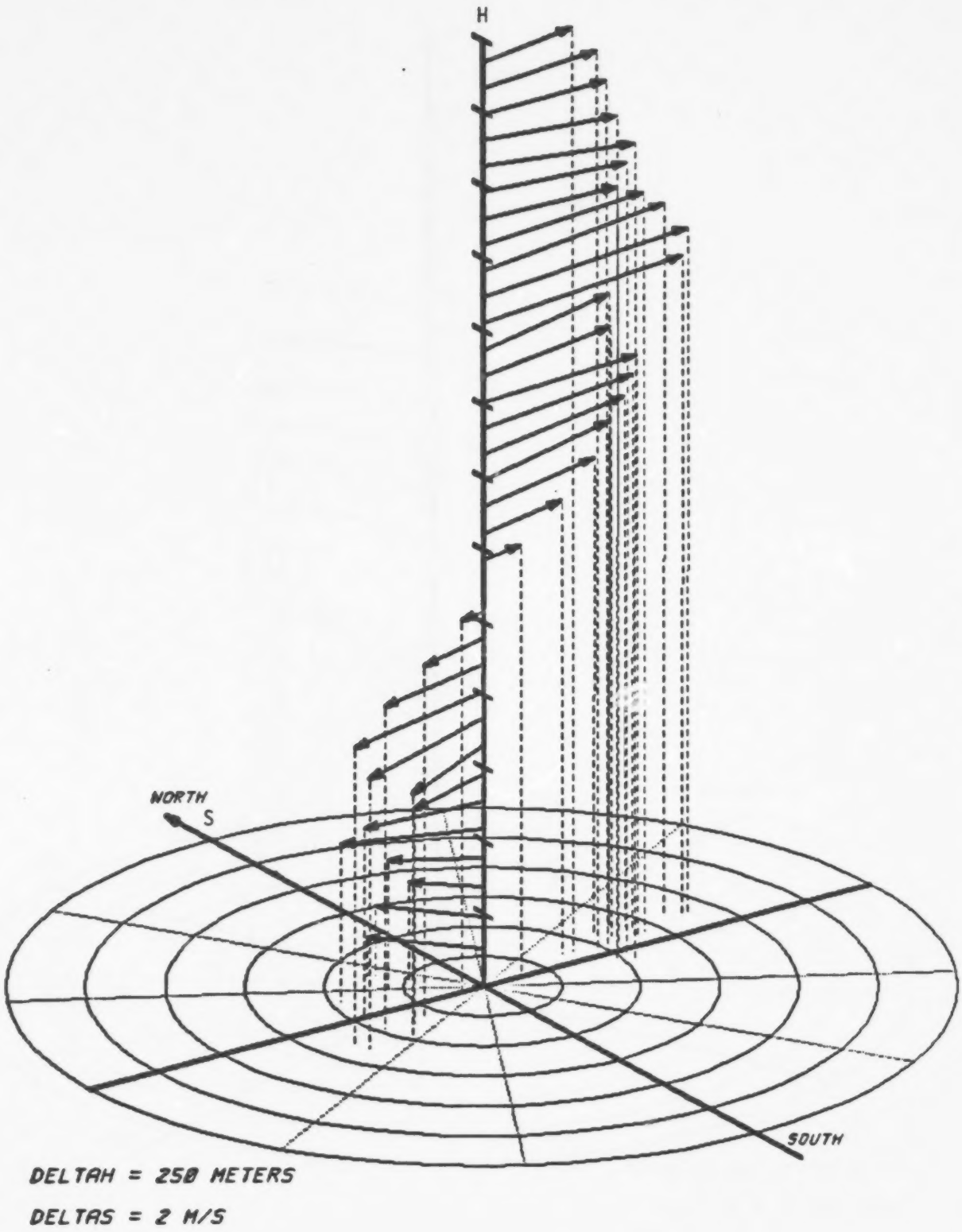

FIGURE A-1. Pibal sounding at Wilmington, Delaware on 19 July 1979, 1200 EST.

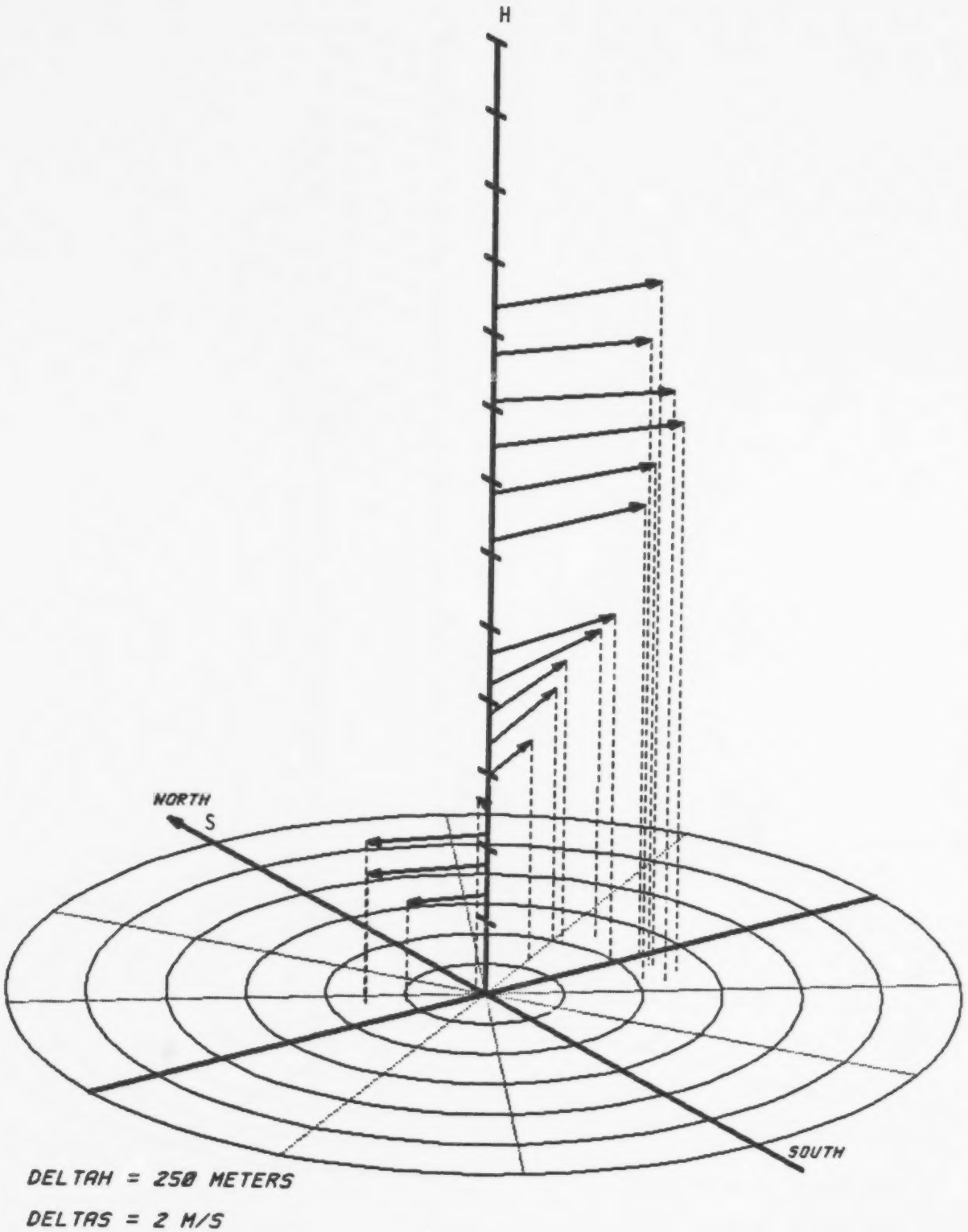

FIGURE A-2. Pibal sounding at Philadelphia, Pennsylvania on 19 July 1979, 1150 EST.

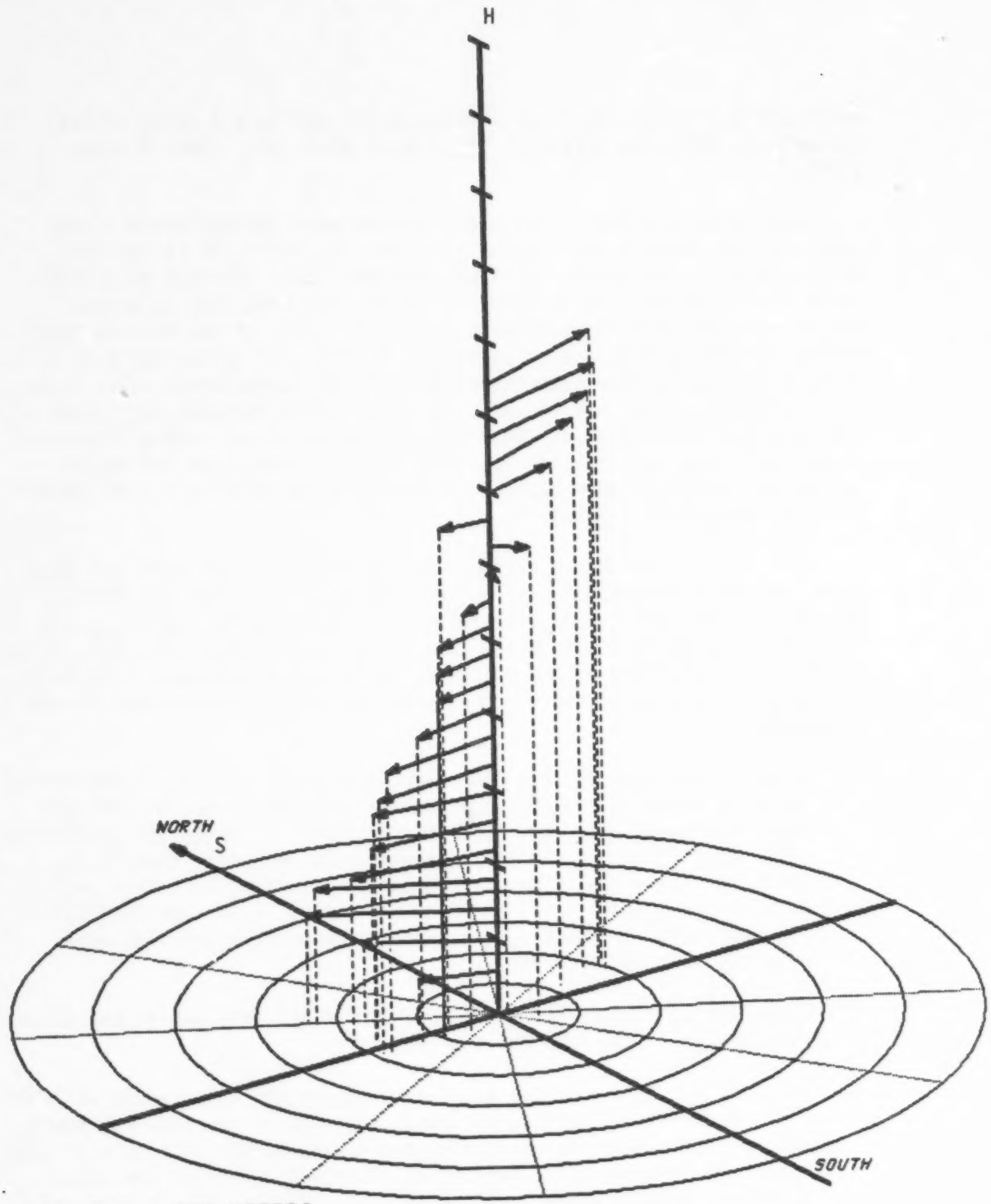

FIGURE A-3. Pibal sounding at Trenton, New Jersey on 19 July 1979, 1300 EST.

overnight mixing heights in Philadelphia, St. Louis, and other cities (Godowitch, 1984; Godowitch, et al., 1984b; Bornstein, 1968; Clarke, 1969).

Mixing heights during the evening transition between convectively dominated and mechanically dominated mixing are difficult to estimate, particularly in the absence of local measurements. In order to approximate this transition so as to avoid sharp discontinuities in mixing height in a manner consistent with the capabilities of the Airshed Model, mixing heights were decreased at a rate of ~2-3 m/min after the time of maximum average surface temperature at 1400 EST (Noonkester, 1976; Kaimal, et al., 1982). This rate was used for urban mixing heights until 2300 EST when the overnight value of 250 m was assumed to be applicable. In rural areas, this rate was applied until 1800 EST, at which time the mixing height was decreased more rapidly to reach the overnight value of 100 m by 2000 EST (Godowitch, 1984b).

For 19 July the hourly averaged mixing height values were estimated using available radiosonde observations and sodar data for the Philadelphia area. The radiosondes were released in downtown Philadelphia; the sodar was located at Summit Bridge, Delaware. Both urban and rural mixing heights were specified on the half hour beginning at midnight. The following procedures were used in specifying the mixing heights used in the simulation:

Urban mixing heights from 0500 through 1500 EST were estimated using vertical potential temperature profiles obtained from Philadelphia upper-air soundings. For each hour, the mixing height was considered to be at the base of the layer in which the potential temperature increased rapidly with height. Upper-air sounding data were available from the urban site for 0500, 0714, 0937, 1150, and 1500 EST. For hours between soundings, potential temperature profiles were obtained by interpolation;

Urban mixing heights between 0000 and 0500 EST were set at the value estimated from the 0500 EST sounding;

The data indicate that the maximum mixing height was reached at 1200 EST. Urban mixing heights following the time of the 1500 EST sounding were determined by decreasing the mixing height at a rate of ~2-3 m/min (Noonkester, 1976; Kaimal, et al., 1982) to reach the 250-m overnight default value by 2100 EST.

Other Meteorological Inputs

Six meteorological scalars that vary in time only are required as inputs to the Urban Airshed Model. Information needed to calculate each scalar is contained in the routinely collected meteorological data. In this study, the temperature gradient above and below the inversion was calculated from the rawinsonde data. A value of 24000 ppm was specified for the concentration of water for both days. The atmospheric pressure was set to 1.0 atm for both days.

The exposure class categories chosen for each hour were specified after reviewing the available meteorological data including surface temperatures, solar radiation data, and synoptic weather summaries. As detailed in Braverman and Haney (1985), the exposure class is a measure of near ground-level stability due to surface heating or cooling and can be estimated from insolation as follows:

$$\text{exposure class} = \begin{cases} 3, \text{strong} \\ 2, \text{moderate} \\ 1, \text{slight} \end{cases} \text{daytime insolation}, \quad \begin{cases} 0, \text{heavy overcast} & \text{day or night} \\ -1, > \frac{4}{8} \text{ cloud cover} \\ -2, < \frac{3}{8} \text{ cloud cover} \end{cases} \text{nighttime cloudiness.}$$

The exposure class categories chosen for each hour were specified after reviewing the available meteorological data including surface temperatures, solar radiation data, and synoptic weather summaries for both days.

A computer program developed by Schere and Demerjian (1977) was used to calculate layer-averaged NO_2 photolysis rate constants based on month, day, year, latitude, longitude, time zone, time of day, mixing height, and measured solar radiation data. The first seven parameters were used to calculate zenith angles and corresponding clear sky theoretical surface NO_2 photolysis rate constants. The mixing heights, along with the parameters used to calculate clear sky theoretical surface NO_2 photolysis rate constants, were used in the calculation of clear sky theoretical layer-averaged NO_2 photolysis rate constants. The methodology used to determine the theoretical surface and layer-averaged NO_2 photolysis rate constants is described by Demerjian et al. (1980). The total measured

solar radiation data in langley/min was multiplied by the constant 0.40 min^{-1} min/langley derived by Jeffries et al. (1982) to convert the solar radiation data to empirical surface NO_2 photolysis rate constants (min^{-1}). The empirical layer-averaged NO_2 photolysis rate constant was calculated by the following equation:

$$\text{Empirical layer-averaged } NO_2 \text{ photolysis rate constant} = \frac{\text{Empirical surface } NO_2 \text{ photolysis rate constant}}{\text{Clear sky theoroetical surface } NO_2 \text{ photolysis rate constant}} \times \text{Clear sky theoretical layer-averaged } NO_2 \text{ photolysis rate constant}$$

A complete set of inputs used in the METSCALARS file for 13 July and 19 July is contained in Tables A-1 and A-2.

EMISSIONS INPUTS

The gridded minor point, area, mobile, and elevated point source emission inventory was prepared for the EPA in 1981 by Engineering Science, Inc., (EPA, 1982). (The boundary of the gridded inventory is shown in Figure A-4.) The bold line defines the area for which gridded emission estimates were available for the 1979 inventory. Hourly (local daylight time) emission values for total NO_x and total hydrocarbon are presented in Table A-3. Total daily emissions by source type are presented in Table A-4 for NO, NO_2, and hydrocarbons. This table also gives the average hydrocarbon splits for the entire emissions inventory. The gridded spatial distribution of ground-level hydrocarbon emissions is presented in Figure A-5. The gridded spatial distribution of ground-level NO_x emissions is presented in Figure A-6.

TERRAIN

The terrain of the modeling region was classified according to land-use values estimated while compiling the emission inventory (EPA, 1982). For grid squares not contained in the emission inventory region, land-use classifications were obtained from a United States Geological Survey (USGS) map with a 1:250,000 scale. Each land-use category was assigned a surface roughness value and an estimate of surface uptake velocity (vegetation factor) according to Wesely (1983) (Table A-5). Land-use classification by grid cells for the Philadelphia modeling region is presented in Figure A-7.

TABLE A-1. METSCALAR FILE FOR THE 13 JULY 1979 AIRSHED SIMULATION

Hour (EST)	Temp. Gradient (°K/m) Above	Temp. Gradient (°K/m) Below	Exposure Class	NO_2 Photolysis Rate (RADFACTOR)	Water Concentration (ppm)	Atmospheric Pressure (atm)
0000-0100	-0.006	-0.000	0	--	24,000	1.0
0100-0200	-0.006	-0.000	0	--	24,000	1.0
0200-0300	-0.006	-0.000	0	--	24,000	1.0
0300-0400	-0.006	-0.000	0	--	24,000	1.0
0400-0500	-0.006	-0.000	0	0.005	24,000	1.0
0500-0600	-0.006	-0.010	1	0.067	24,000	1.0
0600-0700	-0.006	-0.010	1	0.150	24,000	1.0
0700-0800	-0.006	-0.010	1	0.264	24,000	1.0
0800-0900	-0.006	-0.010	2	0.404	24,000	1.0
0900-1000	-0.006	-0.010	2	0.512	24,000	1.0
1000-1100	-0.006	-0.010	2	0.543	24,000	1.0
1100-1200	-0.006	-0.010	3	0.550	24,000	1.0
1200-1300	-0.006	-0.010	3	0.547	24,000	1.0
1300-1400	-0.006	-0.010	3	0.479	24,000	1.0
1400-1500	-0.006	-0.010	3	0.393	24,000	1.0
1500-1600	-0.006	-0.010	3	0.263	24,000	1.0
1600-1700	-0.006	-0.010	2	0.095	24,000	1.0
1700-1800	-0.006	-0.010	2	0.027	24,000	1.0
1800-1900	-0.006	-0.000	1	0.015	24,000	1.0
1900-2000	-0.006	-0.000	1	--	24,000	1.0
2000-2100	-0.006	-0.000	0	--	24,000	1.0
2200-2300	-0.006	-0.000	0	--	24,000	1.0
2300-2400	-0.006	-0.000	0	--	24,000	1.0

TABLE A-2. METSCALAR INPUTS FOR THE 19 JULY 1979 SIMULATION

Hour (EST)	Temp. Gradient (°K/m) Concen-Above	Below	Atmospheric Class	Rate (RADFACTOR)	Exposure tration (ppm)	NO_2 Photolysis Water Pressure (atm)
0000-0100	+0.004	-0.005	0.0	0.000	24,000	1.0
0100-0200	+0.004	-0.005	0.0	0.000	24,000	1.0
0200-0300	+0.004	-0.005	0.0	0.000	24,000	1.0
0300-0400	+0.004	-0.005	0.0	0.000	24,000	1.0
0400-0500	+0.004	-0.005	0.0	0.000	24,000	1.0
0500-0600	+0.004	-0.009	1.0	0.050	24,000	1.0
0600-0700	+0.040	-0.009	1.0	0.147	24,000	1.0
0700-0800	-0.005	-0.009	1.0	0.290	24,000	1.0
0800-0900	-0.005	-0.009	2.0	0.410	24,000	1.0
0900-1000	-0.005	-0.011	2.0	0.483	24,000	1.0
1000-1100	-0.005	-0.011	2.0	0.499	24,000	1.0
1100-1200	-0.007	-0.011	3.0	0.497	24,000	1.0
1200-1300	-0.007	-0.011	3.0	0.487	24,000	1.0
1300-1400	-0.007	-0.011	3.0	0.453	24,000	1.0
1400-1500	-0.007	-0.011	3.0	0.387	24,000	1.0
1500-1600	-0.008	-0.011	3.0	0.279	24,000	1.0
1600-1700	-0.008	-0.011	2.0	0.192	24,000	1.0
1700-1800	-0.005	-0.009	2.0	0.109	24,000	1.0
1800-1900	-0.005	-0.009	1.0	0.019	24,000	1.0
1900-2000	-0.005	-0.009	1.0	0.000	24,000	1.0
2000-2100	-0.005	-0.009	0.0	0.000	24,000	1.0
2100-2200	+0.004	-0.005	0.0	0.000	24,000	1.0
2200-2300	+0.004	-0.005	0.0	0.000	24,000	1.0
2300-2400	+0.004	-0.005	0.0	0.000	24,000	1.0

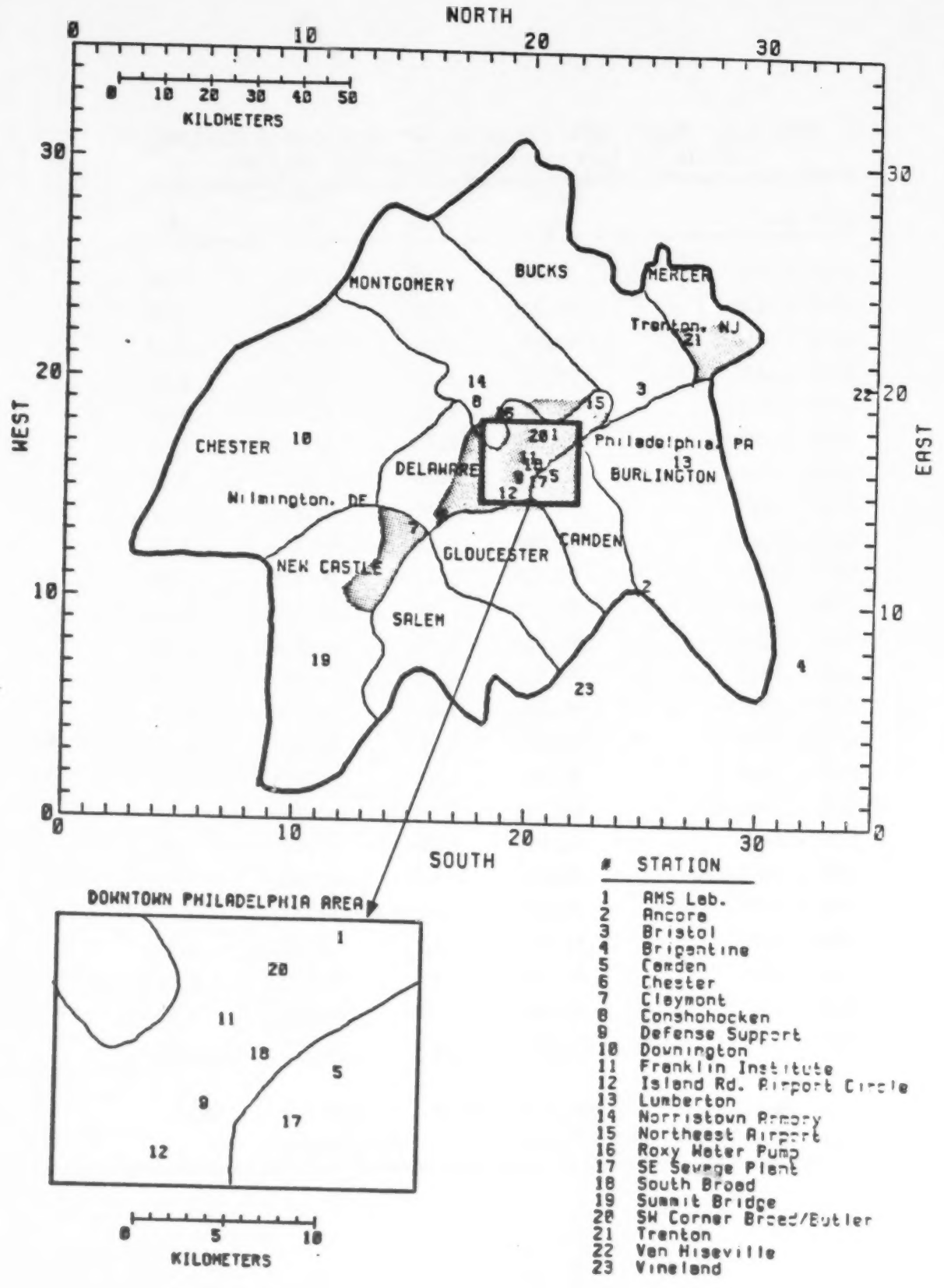

FIGURE A-4. Philadelphia airshed modeling region.

TABLE A-3. HOURLY EMISSIONS OF NO_x AND HYDROCARBON (TONS/HR) USED IN THE 1979 PHILADELPHIA EMISSION INVENTORY

Hour (LDT)	Total NO_x	%	Total HC	%
0000 - 0100	23.413	2.50	17.255	1.42
0100 - 0200	21.070	2.25	15.090	1.24
0200 - 0300	19.886	2.13	12.413	1.02
0300 - 0400	19.712	2.11	11.777	0.97
0400 - 0500	20.461	2.19	11.444	0.94
0500 - 0600	24.625	2.63	14.422	1.18
0600 - 0700	33.658	3.60	25.677	2.11
0700 - 0800	53.234	5.70	81.214	6.67
0800 - 0900	53.623	5.74	94.468	7.76
0900 - 1000	49.794	5.33	89.978	7.39
1000 - 1100	50.629	5.42	89.809	7.37
1100 - 1200	51.720	5.53	84.016	6.90
1200 - 1300	46.660	4.99	77.34	6.35
1300 - 1400	50.451	5.40	75.132	6.17
1400 - 1500	51.662	5.53	75.917	6.23
1500 - 1600	54.883	5.87	81.869	6.72
1600 - 1700	58.815	6.29	74.434	6.11
1700 - 1800	52.584	5.63	67.097	5.51
1800 - 1900	42.650	4.56	56.362	4.63
1900 - 2000	35.866	3.84	39.228	3.22
2000 - 2100	32.448	3.47	35.537	2.92
2100 - 2200	30.728	3.29	33.102	2.72
2200 - 2300	29.480	3.15	31.363	2.58
2300 - 2400	26.664	2.85	22.956	1.88
Total (tons/day)	934.718	100.0	1217.897	100.0
Total (tons/year)	341,172.000		444,532.000	

TABLE A-4. TOTAL DAILY EMISSIONS BY SOURCE TYPE (g·mole) IN THE 1979 PHILADELPHIA INVENTORY

Source	NO	NO_2	ETH	OLE	PAR	CARB	ARO
Elevated Point	5,738,955	257,086	12,144	7,792	901,823	570,765	139,960
Minor Point	2,041,679	114,837	385,284	183,632	15,846,729	818,880	510,799
Area Source	2,705,097	207,808	295,258	194,471	26,841,693	1,669,555	491,833
Mobile Source	6,646,688	738,496	827,355	664,553	11,635,952	1,337	495,926
Total	17,132,419	1,318,227	1,520,041	1,050,448	55,226,197	4,396,897	1,638,518

Total HC = 63,832,101 Total NO_x = 18,450,646

Philadelphia Hydrocarbon Splits

Species	Carbon-Bond Fraction (% as Carbon)
PAR	74.0
OLE	2.8
ETH	4.1
ARO	13.2
CARB	5.9

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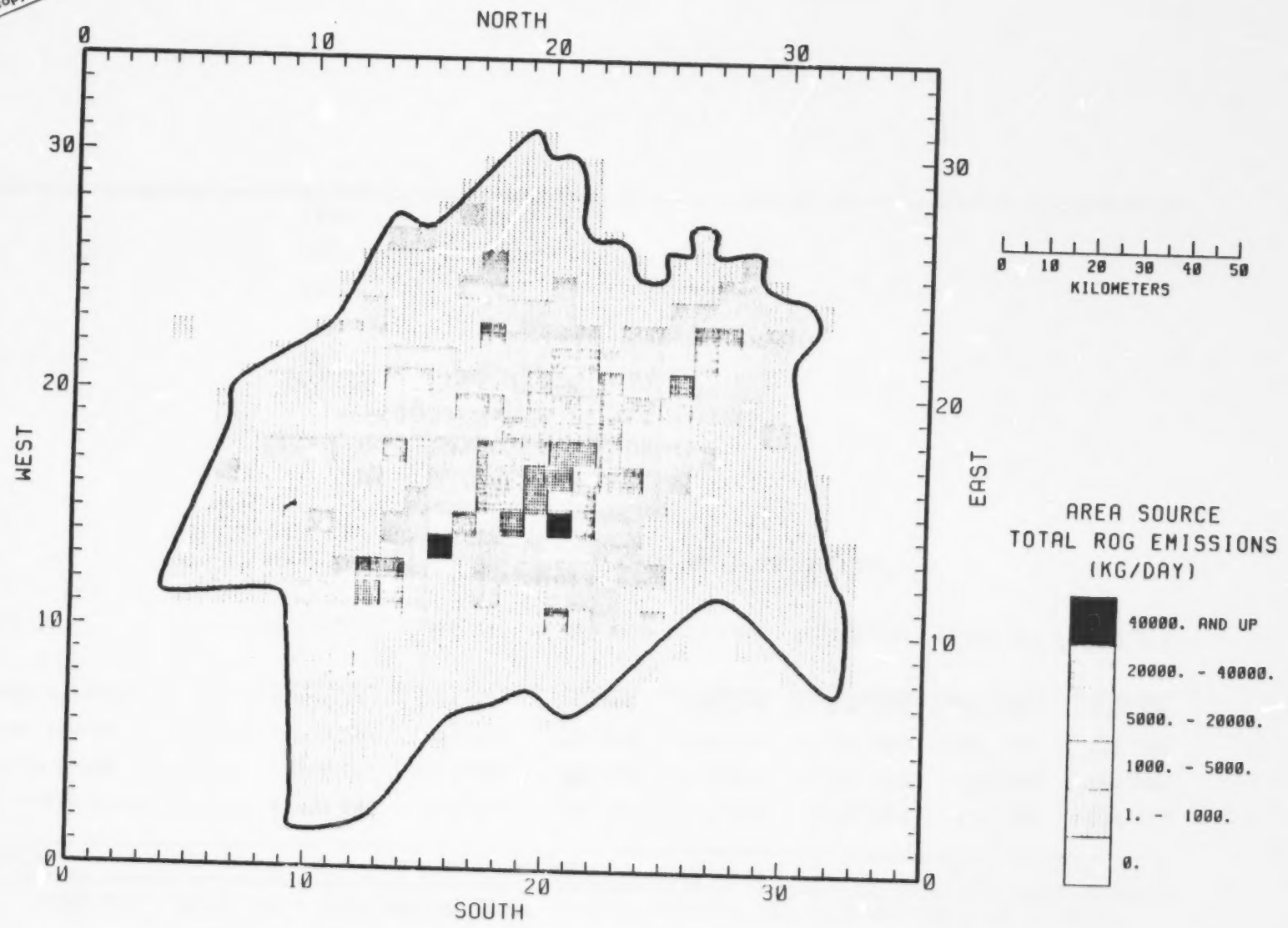

FIGURE A-5. Surface layer total hydrocarbon emissions for the Philadelphia airshed region for 1979.

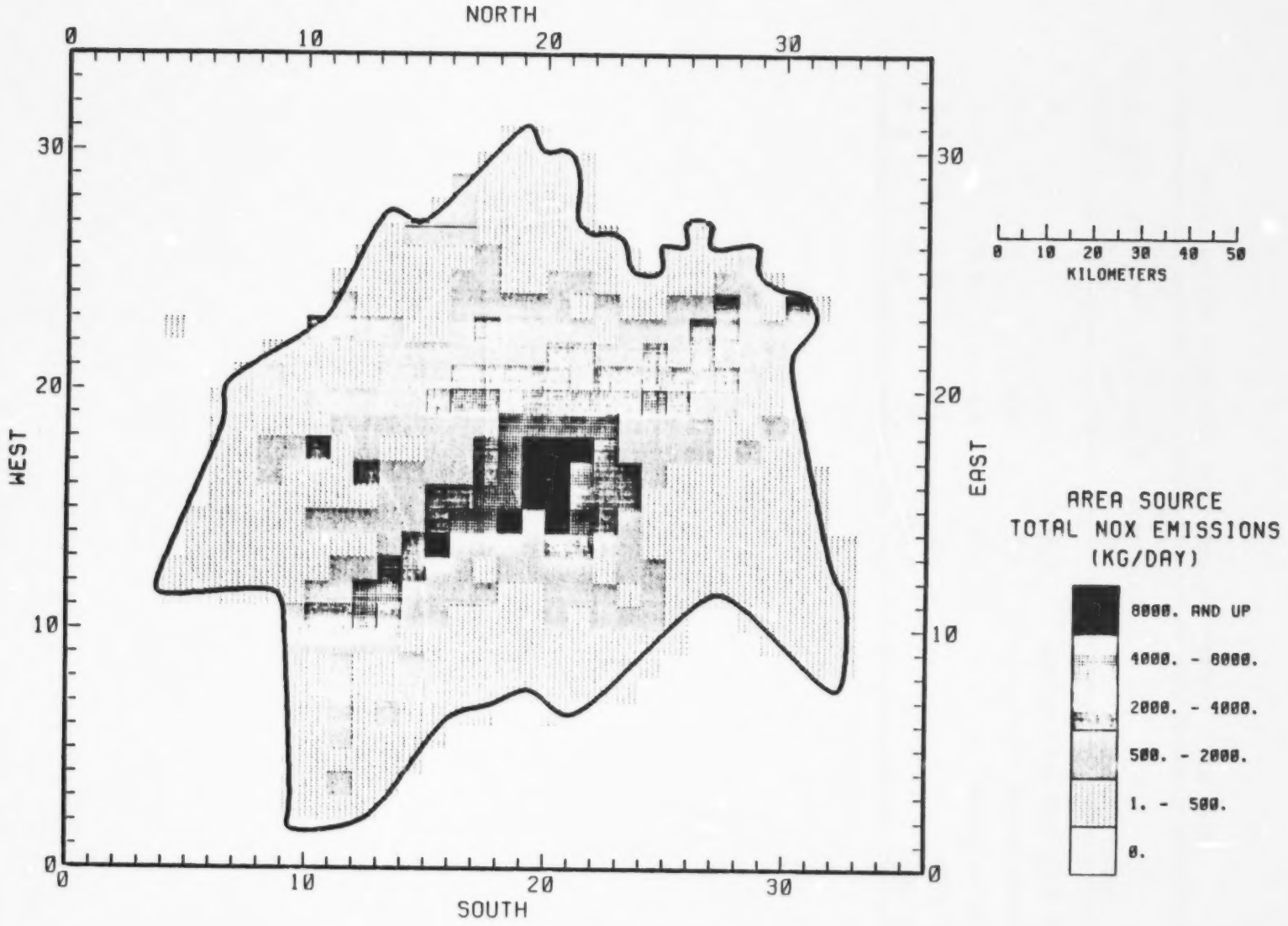

FIGURE A-6. Surface layer total NO_x emissions for the Philadelphia airshed region for 1979.

TABLE A-5. SURFACE ROUGHNESS AND VEGETATION FACTOR VALUES

Land-Use Category	Surface Roughness (m)	Surface Resistance (s/cm)	Uptake Velocity (cm/s)	Vegetation Factor
Mixed Grassland and Cropland	0.10	1.0	1.0	1.0
Deciduous Forest	1.0	0.6	1.7	1.7
Coniferous Forest	1.0	1.5	0.7	0.7
Urban Area	1.0	3.0	0.3	0.3
Ocean Water	0.001	20	0.05	0.05

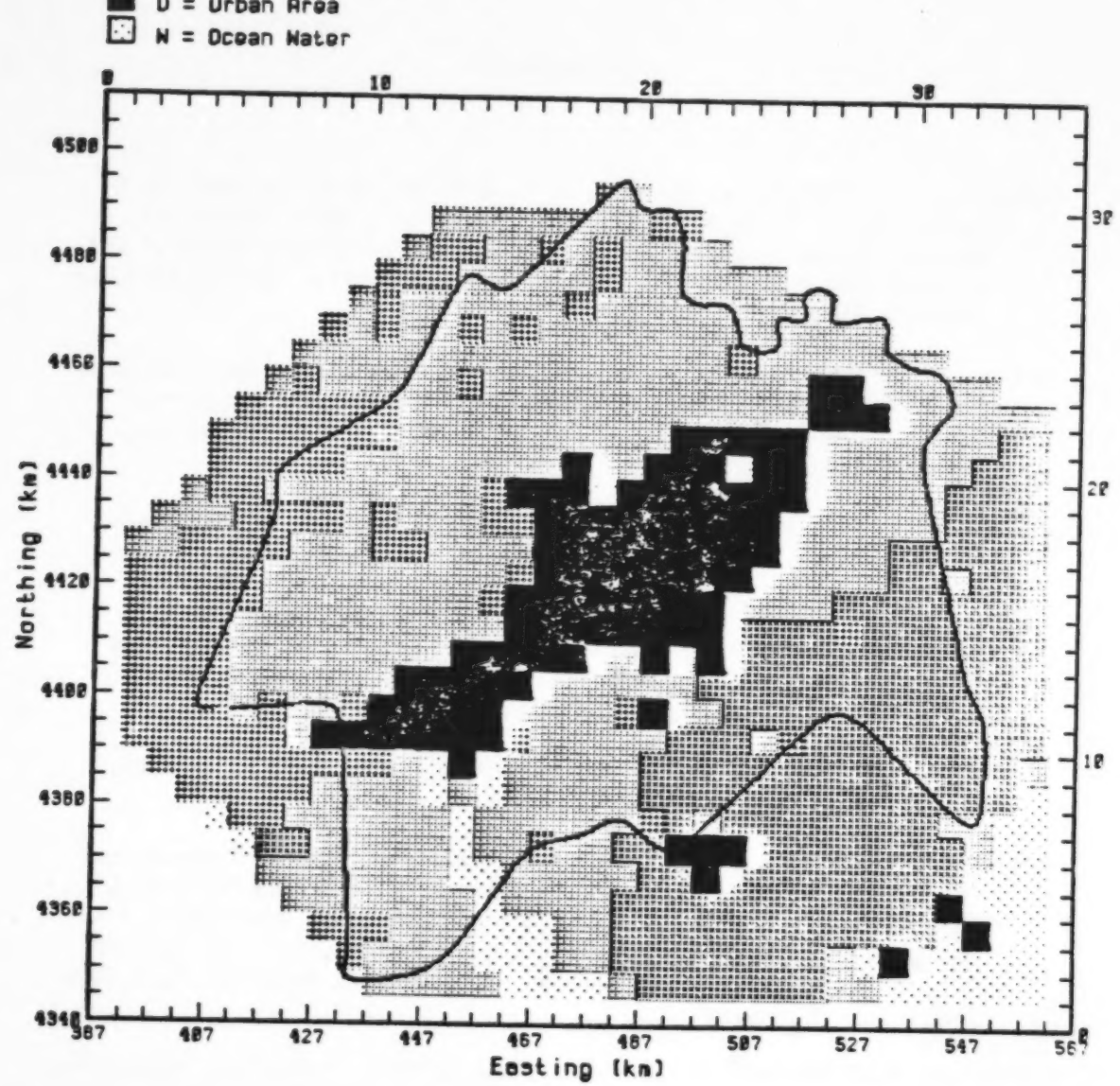

FIGURE A-7. Land-use classifications for the Philadelphia airshed modeling region.

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